



Full wwPDB EM Validation Report ⓘ

Jun 29, 2026 – 02:26 PM EDT

PDB ID : 9OKD / pdb_00009okd
EMDB ID : EMD-70560
Title : Structure of the monomeric Bombyx mori CCAN bound to linear DNA
Authors : Yatskevich, S.; Ciferri, C.
Deposited on : 2025-05-09
Resolution : 2.83 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

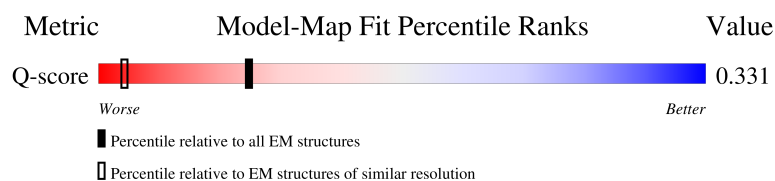
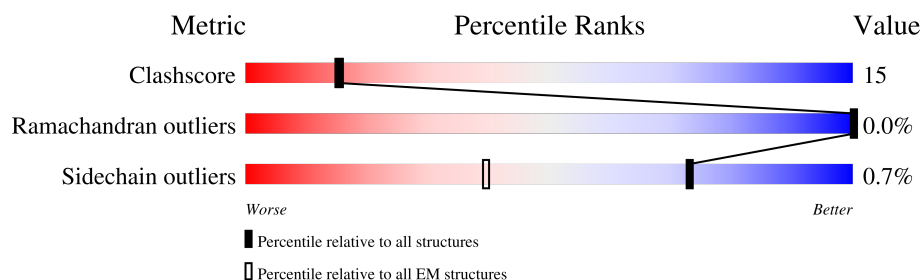
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



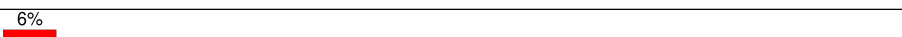
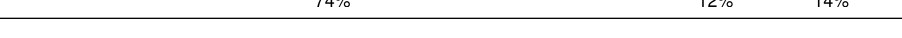
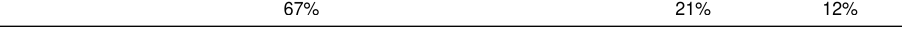
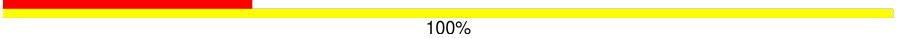
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	239	 69% 26% 5%
2	K	219	 78% 16% • 5%
3	I	661	 71% 17% 12%
4	M	180	 74% 16% 9%

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Mol	Chain	Length	Quality of chain
5	L	302	
6	N	328	
7	O	325	
8	P	638	
9	T	1016	
10	A	95	
11	C	72	
12	D	81	
13	B	82	
14	G	36	
15	J	36	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 42619 atoms, of which 19528 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called bmCENP-H.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	H	228	Total	C	H	N	O	S	0	0
			3517	1170	1666	326	345	10		

- Molecule 2 is a protein called bmCENP-K.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	K	209	Total	C	H	N	O	S	0	0
			3301	1030	1650	273	338	10		

- Molecule 3 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	I	581	Total	C	H	N	O	S	0	0
			9499	3056	4784	788	850	21		

- Molecule 4 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	M	163	Total	C	H	N	O	S	0	0
			2635	818	1349	225	240	3		

- Molecule 5 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	239	Total	C	H	N	O	S	0	0
			3880	1237	1974	309	353	7		

- Molecule 6 is a protein called bmCENP-N.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	N	322	Total	C	H	N	O	S	0	0
			5125	1615	2580	442	476	12		

- Molecule 7 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	O	254	Total	C	H	N	O	S	0	0
			3716	1300	1666	356	381	13		

- Molecule 8 is a protein called bmCENP-P.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	281	Total	C	H	N	O	S	0	0
			4051	1407	1826	371	435	12		

- Molecule 9 is a protein called bmCENP-T.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	155	Total	C	N	O	S	0	0
			1309	842	233	229	5		

- Molecule 10 is a protein called CS-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A	70	Total	C	H	N	O	S	0	0
			1073	341	527	94	108	3		

- Molecule 11 is a protein called DASH complex subunit DAD4.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	C	62	Total	C	H	N	O	S	0	0
			1044	323	517	101	100	3		

- Molecule 12 is a protein called CS-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	D	71	Total	C	H	N	O	S	0	0
			1135	346	570	108	110	1		

- Molecule 13 is a protein called CS-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	55	Total	C	H	N	O	0	0
			858	280	419	75	84		

- Molecule 14 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	36	Total	C	N	O	P	0	0
			739	349	137	217	36		

- Molecule 15 is a DNA chain called DNA (36-MER).

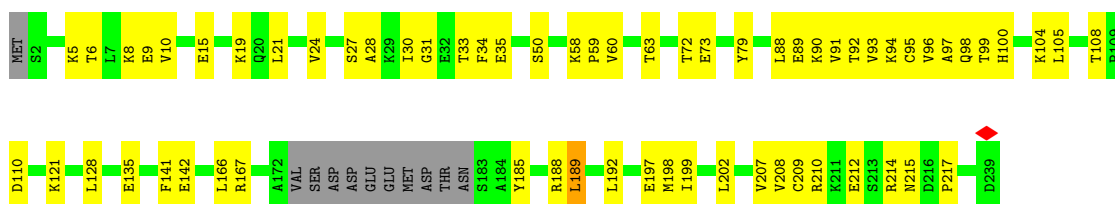
Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	36	Total	C	N	O	P	0	0
			737	348	138	215	36		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

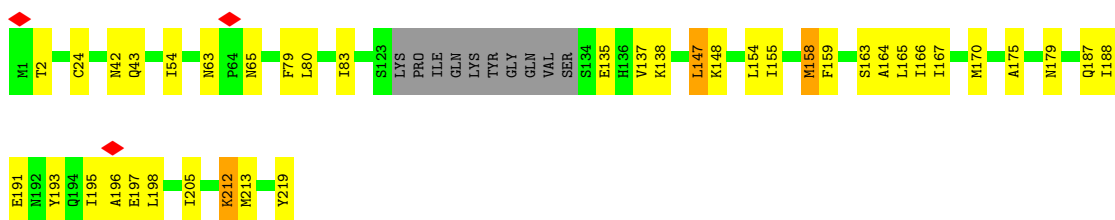
• Molecule 1: bmCENP-H

Chain H: 



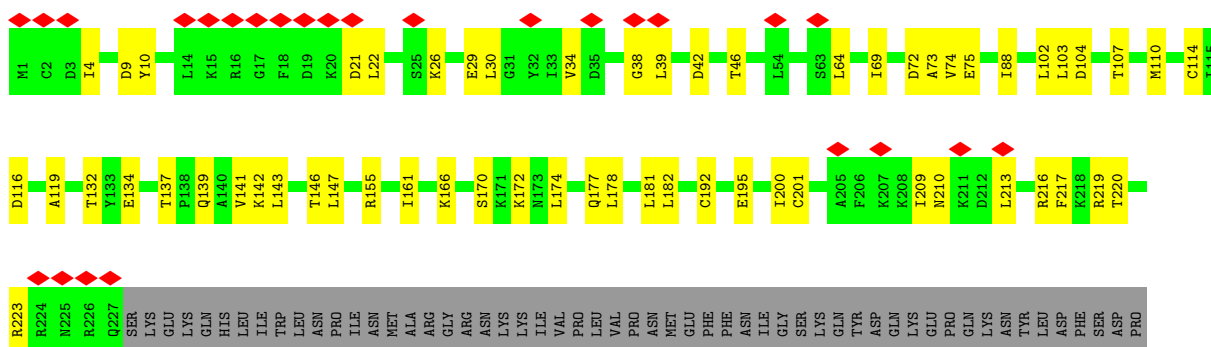
• Molecule 2: bmCENP-K

Chain K: 



• Molecule 3: Centromere protein I

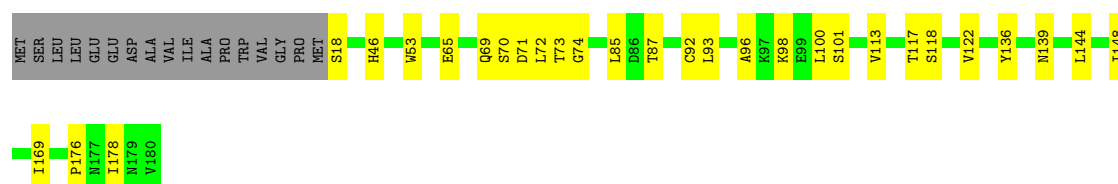
Chain I: 





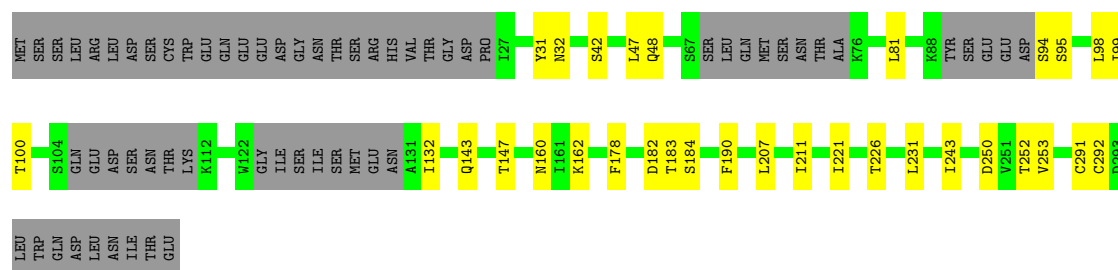
• Molecule 4: Centromere protein M

Chain M: 74% 16% 9%



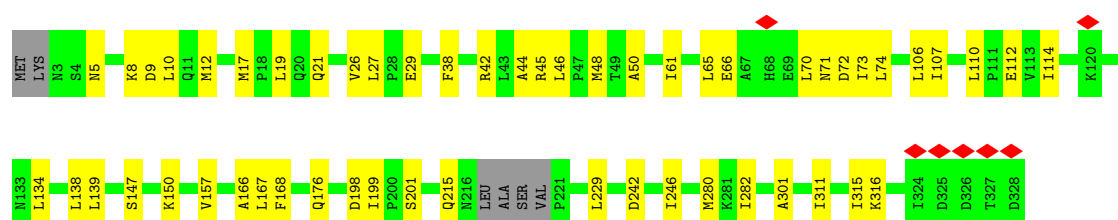
• Molecule 5: Centromere protein L

Chain L: 69% 11% 21%



• Molecule 6: bmCENP-N

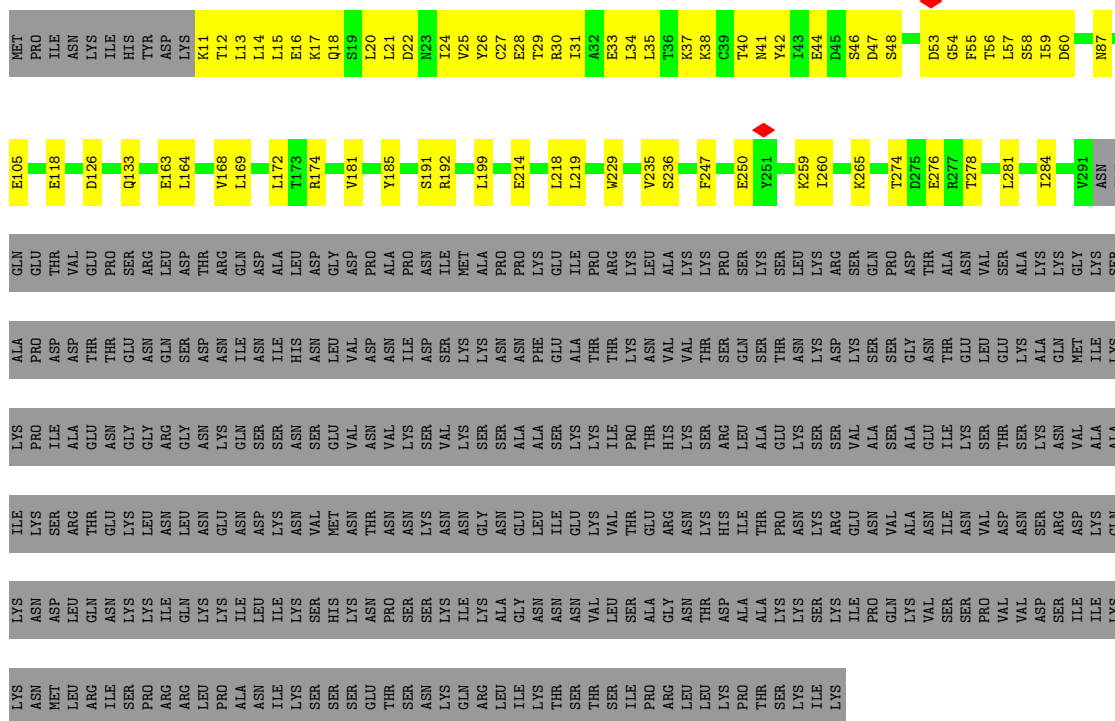
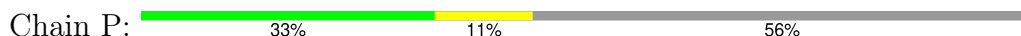
Chain N: 81% 17% 2%



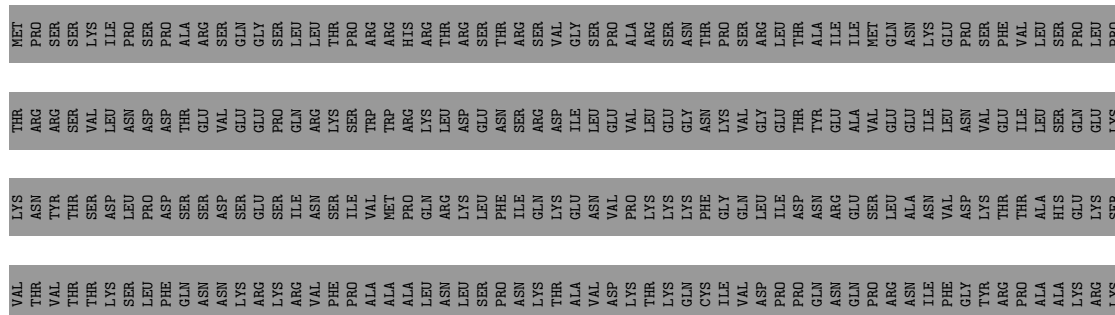
• Molecule 7: Centromere protein O

Chain O: 56% 21% 22%

- Molecule 8: bmCENP-P



- Molecule 9: bmCENP-T



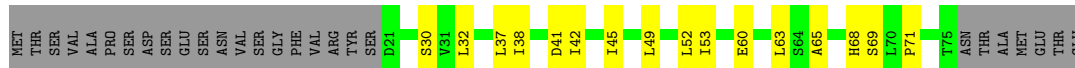
- Molecule 12: CS-4

Chain D: 

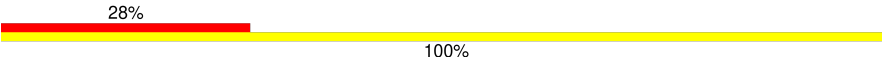


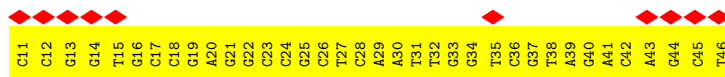
- Molecule 13: CS-2

Chain B: 

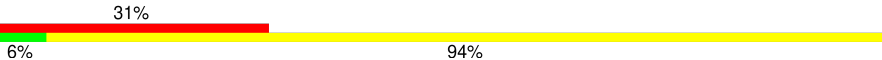


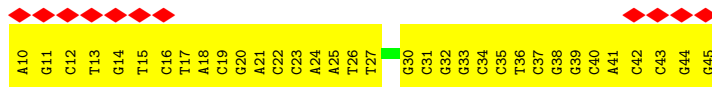
- Molecule 14: DNA (36-MER)

Chain G: 



- Molecule 15: DNA (36-MER)

Chain J: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241975	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.511	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0332	Depositor
Map size (Å)	308.85, 309.575, 309.575	wwPDB
Map dimensions	426, 427, 427	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	H	0.13	0/1872	0.25	0/2508
2	K	0.12	0/1670	0.24	0/2253
3	I	0.11	0/4823	0.23	0/6535
4	M	0.14	0/1302	0.26	0/1764
5	L	0.12	0/1935	0.29	1/2614 (0.0%)
6	N	0.12	0/2594	0.25	0/3516
7	O	0.13	0/2085	0.26	0/2805
8	P	0.12	0/2265	0.27	0/3074
9	T	0.11	0/1339	0.22	0/1797
10	A	0.10	0/548	0.19	0/740
11	C	0.11	0/533	0.19	0/715
12	D	0.15	0/568	0.25	0/761
13	B	0.12	0/446	0.26	0/604
14	G	0.17	0/828	0.35	0/1276
15	J	0.15	0/826	0.30	0/1272
All	All	0.12	0/23634	0.26	1/32234 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	221	ILE	CG1-CB-CG2	5.55	127.36	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1851	1666	1938	59	0
2	K	1651	1650	1658	39	0
3	I	4715	4784	4783	82	0
4	M	1286	1349	1348	21	0
5	L	1906	1974	1969	21	0
6	N	2545	2580	2597	43	0
7	O	2050	1666	2072	74	0
8	P	2225	1826	2241	90	0
9	T	1309	0	1339	147	0
10	A	546	527	572	17	0
11	C	527	517	516	7	0
12	D	565	570	587	15	0
13	B	439	419	453	18	0
14	G	739	0	404	79	0
15	J	737	0	403	52	0
All	All	23091	19528	22880	677	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (677) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:18:DC:H2''	14:G:19:DG:H5''	1.46	0.98
9:T:978:HIS:HA	9:T:986:ARG:HD3	1.48	0.94
14:G:20:DA:H2''	14:G:21:DG:H5'	1.52	0.90
9:T:928:ARG:HH21	9:T:964:LEU:HD11	1.38	0.89
8:P:57:LEU:HD22	8:P:59:ILE:HD11	1.57	0.86
9:T:817:LYS:HE2	9:T:817:LYS:HA	1.58	0.85
14:G:19:DG:H2'	14:G:20:DA:C8	2.10	0.85
9:T:967:VAL:HB	9:T:972:ASP:HB2	1.59	0.83
1:H:27:SER:HB2	7:O:56:SER:HA	1.62	0.82
7:O:259:LYS:NZ	7:O:267:ASP:OD2	2.14	0.81
14:G:34:DG:H2''	14:G:35:DT:H71	1.61	0.81
2:K:24:CYS:SG	4:M:18:SER:OG	2.39	0.81
7:O:30:ILE:HB	7:O:34:ARG:HH21	1.47	0.80
3:I:155:ARG:NH1	3:I:192:CYS:SG	2.55	0.79
2:K:135:GLU:OE1	2:K:135:GLU:N	2.16	0.79
1:H:167:ARG:NH1	3:I:314:ALA:O	2.17	0.78
9:T:900:LYS:H	9:T:900:LYS:HD2	1.50	0.77
14:G:20:DA:H2'	14:G:21:DG:C8	2.21	0.76
9:T:984:GLU:OE1	9:T:984:GLU:N	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:45:ASN:ND2	11:C:50:ASN:OD1	2.18	0.75
1:H:79:TYR:OH	4:M:176:PRO:O	2.04	0.75
14:G:35:DT:H2''	14:G:36:DC:C6	2.20	0.75
7:O:36:ASN:O	7:O:39:GLU:HG3	1.86	0.75
14:G:20:DA:H2'	14:G:21:DG:H8	1.51	0.75
15:J:34:DC:H2''	15:J:35:DC:C5	2.21	0.75
7:O:114:ASP:OD1	8:P:174:ARG:NH2	2.20	0.75
7:O:151:GLU:N	7:O:151:GLU:OE1	2.20	0.74
9:T:895:LYS:HG2	9:T:896:ARG:H	1.51	0.74
9:T:967:VAL:HG21	9:T:973:PHE:HB2	1.69	0.73
9:T:947:GLU:HG2	9:T:948:VAL:HG23	1.70	0.73
10:A:41:GLU:OE1	10:A:41:GLU:N	2.20	0.73
15:J:23:DC:H2''	15:J:24:DA:C8	2.22	0.73
15:J:40:DC:H2''	15:J:41:DA:C8	2.23	0.73
7:O:273:VAL:HG13	7:O:274:GLY:H	1.54	0.72
7:O:64:GLU:N	7:O:64:GLU:OE1	2.20	0.72
8:P:105:GLU:N	8:P:105:GLU:OE1	2.23	0.72
15:J:35:DC:H2''	15:J:36:DT:H71	1.70	0.72
7:O:27:GLN:N	7:O:29:GLU:OE1	2.21	0.71
3:I:170:SER:OG	9:T:903:SER:HA	1.90	0.71
14:G:20:DA:H2''	14:G:21:DG:C5'	2.21	0.71
9:T:993:ILE:HD12	9:T:993:ILE:H	1.54	0.71
3:I:34:VAL:HG22	3:I:39:LEU:HD23	1.71	0.71
14:G:33:DG:H4'	14:G:34:DG:OP1	1.89	0.71
6:N:42:ARG:NH2	9:T:890:LYS:O	2.23	0.71
7:O:262:GLN:N	7:O:262:GLN:OE1	2.24	0.70
1:H:15:GLU:O	1:H:19:LYS:HG2	1.89	0.70
9:T:969:THR:N	9:T:972:ASP:OD2	2.19	0.70
15:J:20:DG:H2''	15:J:21:DA:C8	2.26	0.70
7:O:207:GLN:HG2	7:O:279:ILE:HD12	1.72	0.70
14:G:38:DT:H2''	14:G:39:DA:C8	2.27	0.70
3:I:566:ASP:O	3:I:569:SER:OG	2.07	0.70
6:N:280:MET:HE3	6:N:282:ILE:HD11	1.74	0.70
15:J:19:DC:H2''	15:J:20:DG:C8	2.27	0.70
7:O:27:GLN:N	7:O:27:GLN:OE1	2.25	0.69
9:T:818:SER:O	9:T:821:GLU:HG3	1.92	0.69
3:I:75:GLU:N	3:I:75:GLU:OE1	2.25	0.69
15:J:15:DT:H2''	15:J:16:DC:C5	2.27	0.69
1:H:209:CYS:SG	2:K:158:MET:HE2	2.32	0.69
6:N:29:GLU:N	6:N:29:GLU:OE1	2.25	0.69
4:M:73:THR:HA	8:P:59:ILE:HD12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:31:GLU:O	7:O:34:ARG:HG2	1.93	0.69
7:O:212:GLU:OE1	7:O:214:GLU:N	2.26	0.69
14:G:22:DG:H2''	14:G:23:DC:C6	2.28	0.69
15:J:35:DC:C2'	15:J:36:DT:H71	2.22	0.69
3:I:336:ASP:OD1	3:I:337:ILE:N	2.25	0.69
9:T:947:GLU:N	9:T:947:GLU:OE1	2.25	0.68
14:G:42:DC:H2''	14:G:43:DA:C8	2.28	0.68
3:I:132:THR:HB	9:T:983:ARG:HD2	1.74	0.68
7:O:121:HIS:NE2	7:O:172:TYR:OH	2.25	0.68
9:T:943:VAL:HG23	9:T:949:ALA:HA	1.76	0.68
14:G:41:DA:H2''	14:G:42:DC:C6	2.28	0.68
2:K:195:ILE:HD13	9:T:993:ILE:HD11	1.75	0.68
3:I:139:GLN:N	3:I:139:GLN:OE1	2.25	0.68
6:N:147:SER:OG	6:N:150:LYS:O	2.05	0.68
9:T:928:ARG:HE	9:T:964:LEU:HD21	1.58	0.68
9:T:977:PHE:CE2	9:T:989:VAL:HG11	2.28	0.68
7:O:41:GLN:HB3	13:B:68:HIS:CE1	2.28	0.68
6:N:21:GLN:N	6:N:21:GLN:OE1	2.27	0.68
8:P:276:GLU:N	8:P:276:GLU:OE1	2.27	0.68
3:I:360:LEU:O	3:I:440:ARG:NH1	2.27	0.68
14:G:39:DA:H2''	14:G:40:DG:C8	2.29	0.68
8:P:58:SER:O	8:P:59:ILE:HD13	1.93	0.67
1:H:34:PHE:H	8:P:41:ASN:HD21	1.43	0.67
8:P:214:GLU:OE1	8:P:214:GLU:N	2.26	0.67
9:T:822:LYS:HG3	9:T:825:ARG:HH21	1.59	0.67
15:J:21:DA:H2''	15:J:22:DC:C5	2.29	0.67
1:H:185:TYR:CD1	2:K:137:VAL:HG21	2.30	0.67
15:J:11:DG:H2''	15:J:12:DC:C5	2.30	0.66
9:T:921:TYR:CE2	9:T:928:ARG:HG2	2.31	0.66
9:T:831:ARG:O	9:T:835:LYS:HG2	1.96	0.66
1:H:141:PHE:CE1	9:T:830:VAL:HG13	2.31	0.66
7:O:105:CYS:SG	7:O:156:MET:HE1	2.36	0.66
8:P:57:LEU:HD22	8:P:59:ILE:CD1	2.26	0.66
14:G:32:DT:H2''	14:G:33:DG:C8	2.32	0.65
9:T:916:LYS:HD3	9:T:966:ILE:HA	1.77	0.65
14:G:18:DC:H2''	14:G:19:DG:H8	1.61	0.65
2:K:24:CYS:HG	4:M:18:SER:HG	1.40	0.65
12:D:12:GLU:N	12:D:12:GLU:OE1	2.29	0.65
12:D:75:VAL:O	12:D:79:THR:OG1	2.12	0.65
8:P:55:PHE:CZ	8:P:57:LEU:HD12	2.32	0.65
15:J:24:DA:H2''	15:J:25:DA:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:899:PRO:HD2	9:T:902:ALA:HB3	1.79	0.65
9:T:978:HIS:CA	9:T:986:ARG:HD3	2.25	0.65
8:P:247:PHE:CE2	8:P:284:ILE:HD13	2.32	0.65
14:G:15:DT:H2''	14:G:16:DG:N7	2.12	0.65
10:A:29:LEU:HD13	13:B:41:ASP:OD1	1.97	0.65
5:L:182:ASP:OD1	5:L:183:THR:N	2.30	0.65
8:P:15:LEU:HD12	8:P:16:GLU:N	2.10	0.65
9:T:916:LYS:CD	9:T:966:ILE:HA	2.27	0.65
8:P:41:ASN:OD1	8:P:42:TYR:N	2.30	0.64
1:H:217:PRO:HD3	3:I:88:ILE:HD11	1.78	0.64
14:G:40:DG:H2''	14:G:41:DA:N7	2.12	0.64
8:P:11:LYS:O	8:P:14:LEU:HG	1.97	0.64
8:P:16:GLU:O	8:P:20:LEU:HD23	1.98	0.64
9:T:939:PHE:CG	9:T:957:LEU:HD12	2.33	0.64
14:G:18:DC:C2'	14:G:19:DG:H5''	2.25	0.64
1:H:207:VAL:HG13	1:H:208:VAL:HG13	1.80	0.64
10:A:21:LEU:O	10:A:25:ILE:HG13	1.98	0.64
7:O:29:GLU:O	7:O:33:LEU:HD23	1.98	0.64
7:O:196:ASP:CG	7:O:196:ASP:O	2.41	0.64
8:P:59:ILE:HG22	8:P:60:ASP:H	1.63	0.64
8:P:260:ILE:CG2	8:P:284:ILE:HG13	2.27	0.64
8:P:38:LYS:HZ3	8:P:40:THR:HA	1.64	0.63
15:J:39:DG:H2''	15:J:40:DC:C6	2.34	0.63
1:H:189:LEU:HD23	2:K:137:VAL:HG22	1.79	0.63
5:L:47:LEU:HD23	5:L:132:ILE:HG21	1.80	0.63
14:G:12:DC:H2''	14:G:13:DG:C8	2.33	0.63
15:J:22:DC:H2''	15:J:23:DC:C6	2.33	0.63
15:J:38:DG:H2''	15:J:39:DG:C8	2.33	0.63
3:I:566:ASP:OD2	3:I:583:PHE:N	2.32	0.63
8:P:14:LEU:HD12	8:P:15:LEU:N	2.13	0.63
6:N:66:GLU:OE1	6:N:66:GLU:N	2.31	0.63
3:I:34:VAL:HG12	3:I:219:ARG:HH22	1.64	0.63
9:T:824:MET:O	9:T:828:GLN:HG2	1.98	0.63
14:G:23:DC:H2''	14:G:24:DC:C6	2.34	0.63
8:P:57:LEU:HD23	8:P:58:SER:H	1.64	0.63
14:G:17:DC:H2''	14:G:18:DC:C6	2.34	0.63
14:G:36:DC:H2''	14:G:37:DG:C8	2.34	0.63
14:G:31:DT:H2''	14:G:32:DT:H71	1.81	0.62
8:P:21:LEU:HD12	8:P:22:ASP:N	2.15	0.62
9:T:896:ARG:HA	9:T:930:GLU:OE2	1.98	0.62
14:G:20:DA:C2'	14:G:21:DG:H5'	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:39:DG:H2''	15:J:40:DC:C5	2.34	0.62
6:N:9:ASP:OD1	6:N:10:LEU:N	2.32	0.62
14:G:18:DC:H2''	14:G:19:DG:C8	2.35	0.62
15:J:15:DT:H2''	15:J:16:DC:C6	2.34	0.62
8:P:15:LEU:O	8:P:18:GLN:HG3	1.99	0.62
7:O:31:GLU:O	7:O:35:GLU:HG2	1.98	0.62
14:G:24:DC:H2''	14:G:25:DG:H8	1.64	0.62
4:M:70:SER:O	4:M:74:GLY:N	2.32	0.62
8:P:30:ARG:O	8:P:34:LEU:HD23	2.00	0.61
15:J:37:DC:H2''	15:J:38:DG:C8	2.35	0.61
1:H:60:VAL:O	1:H:63:THR:OG1	2.13	0.61
8:P:30:ARG:O	8:P:33:GLU:HG2	1.99	0.61
8:P:281:LEU:O	8:P:284:ILE:HG22	2.00	0.61
1:H:8:LYS:HD2	11:C:23:GLU:OE1	2.01	0.61
1:H:142:GLU:OE1	3:I:528:LYS:NZ	2.17	0.61
9:T:906:THR:O	9:T:907:LYS:HB3	1.99	0.61
9:T:928:ARG:NH1	9:T:931:LYS:HD3	2.15	0.61
1:H:35:GLU:OE1	1:H:35:GLU:N	2.34	0.61
2:K:2:THR:HG21	8:P:41:ASN:HB2	1.83	0.61
14:G:44:DG:H2''	14:G:45:DC:C6	2.36	0.61
9:T:970:HIS:HD2	9:T:1008:ILE:HG12	1.66	0.61
9:T:999:ILE:HD11	9:T:1004:VAL:CG1	2.31	0.61
8:P:18:GLN:HA	8:P:21:LEU:CD2	2.31	0.60
14:G:13:DG:H2''	14:G:14:DG:C8	2.36	0.60
14:G:35:DT:H2''	14:G:36:DC:C5	2.35	0.60
14:G:14:DG:H2'	14:G:15:DT:H72	1.84	0.60
9:T:992:ASP:OD1	9:T:995:ASN:ND2	2.35	0.60
14:G:17:DC:H2''	14:G:18:DC:C5	2.37	0.60
9:T:936:ILE:O	9:T:940:THR:HG23	2.02	0.60
3:I:104:ASP:O	3:I:107:THR:OG1	2.14	0.60
14:G:16:DG:H2''	14:G:17:DC:C6	2.37	0.60
15:J:21:DA:H2''	15:J:22:DC:C6	2.37	0.60
2:K:159:PHE:O	2:K:163:SER:N	2.35	0.59
7:O:29:GLU:HG2	8:P:17:LYS:CE	2.32	0.59
8:P:38:LYS:NZ	8:P:40:THR:HA	2.16	0.59
8:P:57:LEU:HD23	8:P:58:SER:N	2.16	0.59
3:I:658:GLU:OE1	3:I:658:GLU:N	2.34	0.59
14:G:43:DA:H2''	14:G:44:DG:C8	2.37	0.59
3:I:566:ASP:OD2	3:I:584:VAL:N	2.35	0.59
9:T:888:ASP:OD1	9:T:890:LYS:NZ	2.19	0.59
14:G:37:DG:H2'	14:G:38:DT:H72	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:207:GLN:CG	7:O:279:ILE:HD12	2.32	0.59
3:I:627:ASP:OD1	3:I:628:GLU:N	2.35	0.59
14:G:14:DG:H2''	14:G:15:DT:C6	2.38	0.59
7:O:185:LEU:HD12	7:O:185:LEU:O	2.02	0.59
15:J:43:DC:H2''	15:J:44:DG:C8	2.37	0.59
4:M:71:ASP:OD1	4:M:72:LEU:N	2.35	0.59
9:T:940:THR:O	9:T:943:VAL:HG12	2.03	0.59
3:I:174:LEU:O	3:I:178:LEU:HD23	2.03	0.58
6:N:48:MET:H	9:T:893:PRO:HG3	1.68	0.58
7:O:60:LYS:HE2	8:P:48:SER:HA	1.85	0.58
8:P:18:GLN:HA	8:P:21:LEU:HD21	1.84	0.58
8:P:191:SER:OG	8:P:274:THR:HG22	2.03	0.58
1:H:135:GLU:OE2	3:I:522:SER:OG	2.13	0.58
1:H:202:LEU:HD21	2:K:170:MET:CE	2.32	0.58
14:G:29:DA:H2''	14:G:30:DA:C8	2.39	0.58
8:P:229:TRP:CZ3	8:P:281:LEU:HD11	2.39	0.58
14:G:15:DT:H2''	14:G:16:DG:C8	2.37	0.58
15:J:33:DG:H2''	15:J:34:DC:C6	2.38	0.58
3:I:396:ASP:OD1	3:I:397:SER:N	2.37	0.58
7:O:48:GLN:O	7:O:51:SER:OG	2.14	0.58
9:T:977:PHE:CD1	9:T:981:MET:HG3	2.38	0.58
8:P:31:ILE:O	8:P:35:LEU:HG	2.04	0.58
9:T:910:TYR:CE1	9:T:933:VAL:HG21	2.39	0.58
9:T:926:ARG:O	9:T:926:ARG:HD3	2.04	0.58
6:N:112:GLU:N	6:N:112:GLU:OE1	2.35	0.58
7:O:29:GLU:O	7:O:32:LYS:HG2	2.03	0.58
9:T:932:LEU:O	9:T:935:THR:HG22	2.04	0.58
2:K:198:LEU:HD11	9:T:994:VAL:HG23	1.86	0.57
6:N:176:GLN:N	6:N:176:GLN:OE1	2.36	0.57
14:G:24:DC:H2''	14:G:25:DG:C8	2.39	0.57
7:O:29:GLU:HA	7:O:32:LYS:HE2	1.84	0.57
9:T:959:HIS:O	9:T:963:ARG:HG3	2.03	0.57
14:G:19:DG:H2'	14:G:20:DA:O4'	2.03	0.57
9:T:932:LEU:HA	9:T:935:THR:HG22	1.86	0.57
9:T:960:GLU:O	9:T:964:LEU:HD13	2.05	0.57
6:N:138:LEU:HD11	6:N:199:ILE:HG21	1.86	0.57
9:T:825:ARG:O	9:T:829:GLU:HG3	2.05	0.57
3:I:553:HIS:O	3:I:557:ILE:HG12	2.04	0.57
15:J:10:DA:H2''	15:J:11:DG:C8	2.39	0.57
6:N:70:LEU:O	6:N:73:ILE:HG22	2.04	0.57
9:T:928:ARG:NH2	9:T:964:LEU:HD11	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:27:GLN:O	7:O:30:ILE:HG12	2.04	0.57
14:G:44:DG:H2''	14:G:45:DC:C5	2.39	0.57
7:O:60:LYS:HD3	8:P:48:SER:O	2.05	0.57
9:T:948:VAL:HA	9:T:988:LYS:HG3	1.87	0.57
9:T:952:ASP:OD1	9:T:953:ALA:N	2.38	0.57
5:L:253:VAL:HG21	6:N:301:ALA:HB2	1.85	0.56
15:J:44:DG:H2''	15:J:45:DG:C8	2.39	0.56
4:M:65:GLU:OE2	4:M:69:GLN:NE2	2.38	0.56
10:A:42:ILE:O	10:A:46:ILE:HG13	2.04	0.56
14:G:37:DG:H2''	14:G:38:DT:C6	2.40	0.56
15:J:13:DT:H2''	15:J:14:DG:C8	2.41	0.56
1:H:5:LYS:O	1:H:9:GLU:HG2	2.05	0.56
8:P:12:THR:HA	8:P:15:LEU:HD21	1.88	0.56
3:I:220:THR:HG22	3:I:223:ARG:HH21	1.70	0.56
3:I:453:GLU:OE1	3:I:453:GLU:N	2.37	0.56
5:L:250:ASP:OD1	5:L:252:THR:OG1	2.23	0.56
3:I:132:THR:CB	9:T:983:ARG:HD2	2.35	0.56
3:I:170:SER:HG	9:T:903:SER:HA	1.71	0.56
8:P:27:CYS:O	8:P:31:ILE:HG13	2.06	0.56
1:H:212:GLU:O	1:H:215:ASN:ND2	2.39	0.56
7:O:67:VAL:O	10:A:20:GLN:NE2	2.36	0.56
9:T:1004:VAL:HG23	9:T:1005:PHE:CD1	2.40	0.56
2:K:193:TYR:CE2	9:T:1004:VAL:HG11	2.41	0.55
3:I:26:LYS:NZ	3:I:29:GLU:OE2	2.37	0.55
14:G:26:DC:H2'	14:G:27:DT:H72	1.88	0.55
12:D:69:ARG:O	12:D:70:SER:OG	2.16	0.55
1:H:212:GLU:N	1:H:212:GLU:OE1	2.39	0.55
6:N:8:LYS:HG2	6:N:12:MET:HE2	1.89	0.55
5:L:182:ASP:OD1	5:L:184:SER:N	2.38	0.55
1:H:30:ILE:HD12	1:H:31:GLY:H	1.72	0.55
3:I:134:GLU:OE1	3:I:134:GLU:N	2.35	0.55
9:T:900:LYS:HD2	9:T:900:LYS:N	2.19	0.55
9:T:968:LYS:O	9:T:1008:ILE:HG13	2.07	0.55
1:H:141:PHE:CZ	9:T:830:VAL:HG13	2.41	0.55
8:P:12:THR:HA	8:P:15:LEU:CD2	2.37	0.55
8:P:46:SER:O	8:P:47:ASP:HB3	2.07	0.55
9:T:940:THR:O	9:T:944:LYS:HG2	2.06	0.55
15:J:12:DC:H2''	15:J:13:DT:C5	2.42	0.55
4:M:69:GLN:O	4:M:73:THR:HG22	2.07	0.55
8:P:199:LEU:HD11	8:P:281:LEU:HD13	1.89	0.55
9:T:993:ILE:HD12	9:T:993:ILE:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:164:ALA:O	2:K:167:ILE:HG22	2.07	0.54
15:J:42:DC:H2''	15:J:43:DC:C6	2.42	0.54
2:K:197:GLU:OE2	9:T:990:VAL:HG11	2.08	0.54
8:P:18:GLN:O	8:P:21:LEU:HG	2.07	0.54
14:G:34:DG:H2''	14:G:35:DT:C7	2.34	0.54
1:H:28:ALA:HB1	12:D:43:ASN:ND2	2.22	0.54
7:O:32:LYS:HG3	7:O:33:LEU:HD22	1.90	0.54
7:O:55:LYS:HD3	7:O:56:SER:H	1.72	0.54
2:K:2:THR:CG2	8:P:41:ASN:HB2	2.37	0.54
9:T:963:ARG:NH1	9:T:1014:VAL:HG13	2.22	0.54
3:I:636:TRP:O	9:T:816:LYS:NZ	2.40	0.54
1:H:105:LEU:HD21	1:H:121:LYS:HB2	1.90	0.54
2:K:175:ALA:O	2:K:179:ASN:ND2	2.41	0.54
5:L:48:GLN:N	5:L:48:GLN:OE1	2.40	0.54
8:P:59:ILE:HG22	8:P:60:ASP:N	2.23	0.54
9:T:916:LYS:HG2	9:T:966:ILE:HD13	1.90	0.54
7:O:29:GLU:HA	7:O:32:LYS:HG2	1.90	0.54
14:G:25:DG:H2''	14:G:26:DC:C6	2.43	0.54
10:A:33:ILE:HD11	13:B:41:ASP:HB2	1.89	0.53
9:T:921:TYR:CD2	9:T:928:ARG:HG2	2.44	0.53
8:P:172:LEU:HD11	8:P:181:VAL:HG21	1.91	0.53
9:T:944:LYS:HE2	9:T:985:ILE:HD11	1.90	0.53
15:J:40:DC:H2''	15:J:41:DA:N7	2.22	0.53
9:T:977:PHE:CD2	9:T:989:VAL:HG11	2.43	0.53
14:G:31:DT:C2'	14:G:32:DT:H71	2.38	0.53
15:J:16:DC:H2''	15:J:17:DT:C6	2.44	0.53
2:K:147:LEU:HD23	2:K:148:LYS:N	2.24	0.53
7:O:45:PHE:CE2	7:O:49:ARG:HD2	2.43	0.53
9:T:977:PHE:HE2	9:T:989:VAL:HG11	1.72	0.53
8:P:12:THR:O	8:P:15:LEU:HG	2.09	0.53
14:G:22:DG:H2''	14:G:23:DC:H6	1.72	0.53
1:H:33:THR:HA	8:P:41:ASN:OD1	2.09	0.53
7:O:31:GLU:HA	7:O:34:ARG:CD	2.38	0.53
3:I:374:LEU:CD1	3:I:404:ILE:HG23	2.38	0.53
1:H:199:ILE:HB	2:K:147:LEU:HD21	1.92	0.52
8:P:25:VAL:O	8:P:29:THR:HG23	2.09	0.52
1:H:21:LEU:HA	1:H:24:VAL:HG12	1.90	0.52
15:J:41:DA:H2''	15:J:42:DC:C6	2.44	0.52
5:L:143:GLN:O	5:L:147:THR:HG23	2.09	0.52
8:P:54:GLY:O	8:P:56:THR:HG22	2.09	0.52
14:G:28:DC:H2''	14:G:29:DA:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:98:LYS:O	4:M:101:SER:OG	2.23	0.52
9:T:820:MET:SD	9:T:824:MET:HE2	2.49	0.52
15:J:12:DC:H2''	15:J:13:DT:C6	2.43	0.52
2:K:212:LYS:NZ	2:K:213:MET:SD	2.63	0.52
6:N:45:ARG:CD	9:T:894:PRO:HD2	2.40	0.52
8:P:33:GLU:O	8:P:37:LYS:N	2.43	0.52
2:K:159:PHE:CD2	2:K:166:ILE:HD13	2.45	0.52
3:I:21:ASP:OD1	3:I:22:LEU:N	2.42	0.52
7:O:251:GLU:O	7:O:254:THR:HG22	2.10	0.52
15:J:31:DC:H2''	15:J:32:DG:H8	1.75	0.52
3:I:141:VAL:HG21	3:I:177:GLN:HB3	1.92	0.51
12:D:60:LEU:HD21	13:B:71:PRO:HB2	1.91	0.51
7:O:154:ASN:OD1	7:O:155:ILE:N	2.44	0.51
1:H:72:THR:OG1	1:H:73:GLU:N	2.42	0.51
3:I:337:ILE:O	5:L:162:LYS:NZ	2.36	0.51
14:G:30:DA:H2''	14:G:31:DT:C6	2.46	0.51
5:L:81:LEU:HD13	5:L:99:ILE:HG13	1.92	0.51
8:P:18:GLN:HA	8:P:21:LEU:HG	1.92	0.51
8:P:164:LEU:HD11	8:P:185:TYR:CD1	2.46	0.51
6:N:166:ALA:C	6:N:167:LEU:HD12	2.36	0.51
9:T:1007:GLU:HB2	9:T:1010:SER:HB3	1.93	0.51
9:T:890:LYS:HG3	9:T:891:TYR:H	1.75	0.51
7:O:59:VAL:HG11	11:C:37:GLU:OE1	2.11	0.51
7:O:69:PRO:HB3	10:A:16:ILE:HG23	1.92	0.51
7:O:210:VAL:HG12	7:O:211:GLU:H	1.75	0.51
7:O:153:ASP:OD1	7:O:154:ASN:N	2.43	0.50
7:O:223:ASP:O	7:O:232:LYS:N	2.44	0.50
9:T:932:LEU:O	9:T:936:ILE:HG23	2.11	0.50
9:T:972:ASP:O	9:T:975:GLN:HG3	2.10	0.50
15:J:25:DA:H2''	15:J:26:DT:C6	2.46	0.50
8:P:20:LEU:O	8:P:24:ILE:HG12	2.11	0.50
8:P:218:LEU:C	8:P:219:LEU:HD12	2.36	0.50
10:A:63:ASP:OD2	10:A:66:ASN:ND2	2.43	0.50
15:J:12:DC:H2''	15:J:13:DT:H71	1.92	0.50
3:I:309:LEU:O	3:I:309:LEU:HD23	2.11	0.50
6:N:17:MET:HE1	6:N:26:VAL:HG13	1.94	0.50
12:D:32:LEU:O	12:D:32:LEU:HD23	2.11	0.50
14:G:14:DG:C2'	14:G:15:DT:H72	2.41	0.50
15:J:26:DT:H2''	15:J:27:DT:C6	2.46	0.50
3:I:216:ARG:O	3:I:220:THR:HG23	2.12	0.50
6:N:157:VAL:HG22	6:N:168:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:41:ASP:O	13:B:45:ILE:HG13	2.11	0.50
1:H:34:PHE:H	8:P:41:ASN:ND2	2.10	0.50
3:I:424:LEU:HD13	3:I:469:MET:HE3	1.94	0.50
5:L:42:SER:OG	5:L:160:ASN:N	2.37	0.50
14:G:27:DT:H2''	14:G:28:DC:C6	2.46	0.50
1:H:110:ASP:OD1	1:H:121:LYS:NZ	2.35	0.49
14:G:31:DT:H2''	14:G:32:DT:C6	2.47	0.49
3:I:505:LEU:HD22	3:I:540:PHE:HE1	1.77	0.49
8:P:22:ASP:O	8:P:25:VAL:HG12	2.12	0.49
8:P:118:GLU:OE2	8:P:133:GLN:NE2	2.45	0.49
14:G:21:DG:H2''	14:G:22:DG:C8	2.47	0.49
5:L:291:CYS:SG	5:L:292:CYS:N	2.82	0.49
8:P:229:TRP:HZ3	8:P:281:LEU:HD11	1.76	0.49
9:T:912:TYR:HA	9:T:915:ASP:OD2	2.12	0.49
15:J:19:DC:H2''	15:J:20:DG:H8	1.76	0.49
3:I:10:TYR:CZ	3:I:22:LEU:HD22	2.48	0.49
3:I:172:LYS:NZ	14:G:20:DA:OP1	2.45	0.49
3:I:629:ARG:O	3:I:633:ASN:ND2	2.45	0.49
9:T:971:PHE:O	9:T:971:PHE:HD1	1.95	0.49
15:J:32:DG:H2''	15:J:33:DG:C8	2.47	0.49
15:J:32:DG:H2''	15:J:33:DG:H8	1.77	0.49
1:H:31:GLY:HA3	8:P:42:TYR:CE1	2.48	0.49
4:M:87:THR:HG1	4:M:118:SER:HG	1.47	0.49
6:N:42:ARG:CZ	9:T:891:TYR:HB2	2.43	0.49
7:O:59:VAL:O	7:O:61:LYS:NZ	2.38	0.49
9:T:896:ARG:HB3	9:T:910:TYR:CE2	2.48	0.49
3:I:38:GLY:C	3:I:39:LEU:HD22	2.37	0.49
3:I:608:SER:O	3:I:612:HIS:N	2.45	0.49
5:L:98:LEU:C	5:L:98:LEU:HD23	2.38	0.49
14:G:30:DA:H2'	14:G:31:DT:H72	1.95	0.49
3:I:376:LEU:HD12	4:M:122:VAL:HG13	1.94	0.49
9:T:958:LYS:HD3	9:T:973:PHE:CD2	2.48	0.48
2:K:63:ASN:ND2	2:K:65:ASN:OD1	2.46	0.48
9:T:822:LYS:HG3	9:T:825:ARG:NH2	2.28	0.48
9:T:1001:ARG:O	9:T:1001:ARG:HD2	2.14	0.48
14:G:23:DC:H2''	14:G:24:DC:H6	1.75	0.48
15:J:37:DC:H2''	15:J:38:DG:H8	1.77	0.48
3:I:30:LEU:C	3:I:30:LEU:HD23	2.38	0.48
9:T:971:PHE:HD2	9:T:1005:PHE:HE1	1.61	0.48
14:G:19:DG:H2'	14:G:20:DA:H8	1.74	0.48
15:J:34:DC:H2''	15:J:35:DC:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:22:LEU:O	3:I:22:LEU:HD23	2.14	0.48
7:O:28:ASP:HA	7:O:31:GLU:OE1	2.13	0.48
14:G:41:DA:H2"	14:G:42:DC:C5	2.48	0.48
15:J:31:DC:H2"	15:J:32:DG:C8	2.48	0.48
6:N:19:LEU:HD23	6:N:19:LEU:C	2.39	0.48
15:J:11:DG:H2"	15:J:12:DC:C6	2.49	0.48
4:M:85:LEU:O	4:M:117:THR:OG1	2.30	0.48
8:P:260:ILE:HG23	8:P:284:ILE:HG13	1.95	0.48
8:P:274:THR:O	8:P:278:THR:HG23	2.13	0.48
9:T:917:LEU:HD21	9:T:964:LEU:HB3	1.96	0.48
3:I:195:GLU:OE1	3:I:195:GLU:N	2.42	0.48
8:P:18:GLN:HA	8:P:21:LEU:CG	2.43	0.48
15:J:12:DC:H2"	15:J:13:DT:C7	2.44	0.48
1:H:104:LYS:O	1:H:108:THR:OG1	2.30	0.48
3:I:4:ILE:HD13	3:I:39:LEU:CD1	2.43	0.48
9:T:822:LYS:O	9:T:826:ILE:HG12	2.14	0.48
9:T:970:HIS:CE1	9:T:1000:PRO:HB3	2.49	0.48
8:P:260:ILE:HG21	8:P:284:ILE:HG13	1.94	0.48
9:T:921:TYR:O	9:T:924:LYS:HB2	2.14	0.48
9:T:999:ILE:HD12	9:T:1000:PRO:HD2	1.95	0.48
14:G:45:DC:H2"	14:G:46:DT:C6	2.48	0.48
1:H:105:LEU:HD23	1:H:105:LEU:C	2.39	0.47
6:N:282:ILE:HD12	6:N:282:ILE:H	1.79	0.47
9:T:888:ASP:C	9:T:889:MET:HG3	2.39	0.47
9:T:899:PRO:HD2	9:T:902:ALA:CB	2.43	0.47
3:I:64:LEU:C	3:I:64:LEU:HD23	2.40	0.47
6:N:242:ASP:O	6:N:246:ILE:HG12	2.14	0.47
7:O:76:ASN:OD1	13:B:30:SER:OG	2.31	0.47
7:O:199:HIS:O	7:O:199:HIS:ND1	2.47	0.47
3:I:74:VAL:N	3:I:114:CYS:O	2.43	0.47
6:N:19:LEU:HD12	6:N:50:ALA:O	2.14	0.47
15:J:22:DC:H2"	15:J:23:DC:C5	2.49	0.47
8:P:281:LEU:HA	8:P:284:ILE:HG22	1.96	0.47
9:T:948:VAL:HA	9:T:988:LYS:CG	2.45	0.47
1:H:214:ARG:O	3:I:88:ILE:HD13	2.14	0.47
2:K:188:ILE:HG22	2:K:213:MET:O	2.14	0.47
7:O:190:GLN:OE1	7:O:190:GLN:N	2.47	0.47
14:G:11:DC:H2"	14:G:12:DC:C6	2.50	0.47
3:I:374:LEU:HD12	3:I:404:ILE:HG23	1.96	0.47
7:O:210:VAL:HG12	7:O:211:GLU:N	2.29	0.47
9:T:966:ILE:HG22	9:T:967:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:14:GLU:O	10:A:17:THR:OG1	2.28	0.47
1:H:50:SER:OG	4:M:169:ILE:O	2.22	0.47
6:N:132:THR:HG23	6:N:139:LEU:HD11	1.97	0.47
6:N:229:LEU:HD21	8:P:57:LEU:HB3	1.96	0.47
7:O:67:VAL:HG21	7:O:71:LYS:HD2	1.95	0.47
9:T:900:LYS:H	9:T:900:LYS:CD	2.26	0.47
9:T:916:LYS:CG	9:T:966:ILE:HD13	2.45	0.47
9:T:940:THR:HA	9:T:943:VAL:HG12	1.97	0.47
3:I:166:LYS:O	9:T:906:THR:HG21	2.15	0.47
9:T:957:LEU:O	9:T:957:LEU:HD23	2.14	0.47
14:G:11:DC:H2''	14:G:12:DC:C5	2.50	0.47
5:L:190:PHE:HB2	5:L:211:ILE:HD13	1.97	0.47
7:O:67:VAL:HG22	7:O:68:ARG:H	1.80	0.47
12:D:46:VAL:HG22	13:B:63:LEU:HD11	1.97	0.47
14:G:39:DA:H2''	14:G:40:DG:H8	1.78	0.47
3:I:4:ILE:HD13	3:I:39:LEU:HD11	1.96	0.46
6:N:38:PHE:CZ	9:T:889:MET:HA	2.49	0.46
9:T:921:TYR:HE2	9:T:928:ARG:HG2	1.75	0.46
14:G:37:DG:C8	14:G:38:DT:H72	2.49	0.46
15:J:36:DT:H2''	15:J:37:DC:C6	2.50	0.46
8:P:235:VAL:HG23	8:P:236:SER:N	2.30	0.46
9:T:999:ILE:CD1	9:T:1000:PRO:HD2	2.45	0.46
14:G:20:DA:C2'	14:G:21:DG:H2'	2.45	0.46
15:J:42:DC:H2''	15:J:43:DC:C5	2.50	0.46
3:I:30:LEU:O	3:I:34:VAL:HG23	2.15	0.46
9:T:999:ILE:HG13	9:T:1000:PRO:HD2	1.97	0.46
3:I:483:VAL:O	3:I:487:ASN:ND2	2.45	0.46
10:A:46:ILE:HD12	13:B:52:LEU:HD22	1.98	0.46
14:G:38:DT:H2''	14:G:39:DA:N7	2.30	0.46
14:G:16:DG:H2''	14:G:17:DC:C5	2.50	0.46
2:K:166:ILE:HG12	2:K:195:ILE:HD12	1.98	0.46
9:T:918:GLU:N	9:T:919:PRO:HD2	2.30	0.46
10:A:29:LEU:O	10:A:33:ILE:HG13	2.16	0.46
15:J:18:DA:H2''	15:J:19:DC:C6	2.51	0.46
1:H:202:LEU:HD21	2:K:170:MET:HE1	1.96	0.46
14:G:33:DG:H2''	14:G:34:DG:C8	2.51	0.46
15:J:30:DG:H2''	15:J:31:DC:C6	2.51	0.46
5:L:94:SER:OG	5:L:95:SER:N	2.47	0.45
8:P:44:GLU:OE1	8:P:44:GLU:N	2.46	0.45
3:I:622:ALA:HA	9:T:815:ILE:HD11	1.98	0.45
3:I:213:LEU:HD11	3:I:217:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:30:ARG:HD2	8:P:33:GLU:OE2	2.16	0.45
14:G:40:DG:N2	15:J:17:DT:O2	2.50	0.45
7:O:220:LEU:HD12	7:O:235:SER:O	2.16	0.45
14:G:19:DG:C2'	14:G:20:DA:O4'	2.65	0.45
1:H:210:ARG:NH2	9:T:993:ILE:HD13	2.31	0.45
3:I:69:ILE:HD13	3:I:216:ARG:HB3	1.98	0.45
9:T:976:PHE:HA	9:T:979:ASP:OD1	2.17	0.45
1:H:93:VAL:O	1:H:94:LYS:C	2.59	0.45
3:I:431:TYR:HH	3:I:498:HIS:CE1	2.30	0.45
9:T:814:LYS:HD2	9:T:814:LYS:C	2.42	0.45
9:T:890:LYS:HG3	9:T:891:TYR:N	2.32	0.45
9:T:892:LYS:O	9:T:893:PRO:C	2.59	0.45
14:G:37:DG:H2''	14:G:38:DT:H6	1.80	0.45
8:P:12:THR:HA	8:P:15:LEU:HG	1.98	0.45
9:T:928:ARG:NE	9:T:964:LEU:HD21	2.30	0.45
15:J:23:DC:H2''	15:J:24:DA:H8	1.80	0.45
1:H:6:THR:O	1:H:10:VAL:HG23	2.17	0.44
1:H:99:THR:O	1:H:100:HIS:C	2.60	0.44
3:I:350:GLN:O	3:I:354:LEU:HD23	2.17	0.44
3:I:432:ILE:HD12	3:I:497:ALA:HB2	1.98	0.44
4:M:92:CYS:SG	4:M:93:LEU:N	2.89	0.44
9:T:907:LYS:HA	9:T:910:TYR:HB2	1.99	0.44
3:I:72:ASP:OD1	3:I:73:ALA:N	2.47	0.44
6:N:215:GLN:OE1	6:N:215:GLN:N	2.41	0.44
7:O:30:ILE:HB	7:O:34:ARG:NH2	2.24	0.44
9:T:832:ASN:HA	9:T:835:LYS:HG2	1.99	0.44
10:A:62:ILE:HD11	13:B:65:ALA:HB1	2.00	0.44
5:L:31:TYR:O	5:L:32:ASN:OD1	2.36	0.44
6:N:311:ILE:O	6:N:316:LYS:N	2.47	0.44
9:T:826:ILE:O	9:T:830:VAL:HG23	2.17	0.44
9:T:827:GLU:O	9:T:831:ARG:HG2	2.17	0.44
10:A:31:GLN:OE1	11:C:43:LYS:NZ	2.29	0.44
3:I:217:PHE:O	3:I:220:THR:OG1	2.29	0.44
8:P:28:GLU:OE1	8:P:28:GLU:HA	2.16	0.44
8:P:40:THR:HG21	8:P:42:TYR:CE2	2.52	0.44
8:P:53:ASP:CG	8:P:54:GLY:H	2.25	0.44
14:G:26:DC:H2''	14:G:27:DT:C6	2.53	0.44
3:I:209:ILE:HG22	3:I:210:ASN:N	2.32	0.44
6:N:73:ILE:HG23	6:N:74:LEU:N	2.33	0.44
9:T:916:LYS:HE2	9:T:916:LYS:HB2	1.86	0.44
9:T:949:ALA:HB2	9:T:989:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:951:ASN:O	9:T:954:VAL:HG12	2.17	0.44
1:H:94:LYS:O	1:H:95:CYS:C	2.59	0.44
1:H:98:GLN:O	1:H:99:THR:C	2.61	0.44
9:T:947:GLU:O	9:T:988:LYS:HG3	2.17	0.44
2:K:191:GLU:OE1	2:K:191:GLU:N	2.45	0.44
3:I:9:ASP:OD1	3:I:10:TYR:N	2.51	0.44
4:M:136:TYR:CD1	4:M:136:TYR:C	2.96	0.44
8:P:58:SER:C	8:P:59:ILE:HD13	2.43	0.44
3:I:363:ILE:HG22	3:I:365:VAL:HG12	2.00	0.44
7:O:32:LYS:HG3	7:O:33:LEU:CD2	2.47	0.44
14:G:41:DA:H2''	14:G:42:DC:H6	1.78	0.44
1:H:188:ARG:O	1:H:192:LEU:HD23	2.18	0.44
3:I:103:LEU:HD11	3:I:143:LEU:HD13	1.99	0.44
9:T:993:ILE:HG22	9:T:993:ILE:O	2.18	0.44
6:N:198:ASP:OD2	6:N:201:SER:OG	2.28	0.43
9:T:896:ARG:HB3	9:T:910:TYR:CZ	2.53	0.43
1:H:166:LEU:HD23	1:H:166:LEU:C	2.43	0.43
3:I:116:ASP:OD1	3:I:119:ALA:HB3	2.18	0.43
7:O:61:LYS:HE2	7:O:61:LYS:H	1.82	0.43
8:P:37:LYS:HG3	8:P:38:LYS:N	2.33	0.43
8:P:168:VAL:HG22	8:P:168:VAL:O	2.17	0.43
1:H:197:GLU:OE1	2:K:219:TYR:OH	2.34	0.43
8:P:87:ASN:ND2	8:P:126:ASP:OD1	2.50	0.43
14:G:19:DG:H4'	14:G:19:DG:OP1	2.17	0.43
1:H:88:LEU:O	1:H:89:GLU:C	2.61	0.43
3:I:42:ASP:O	3:I:46:THR:HG23	2.19	0.43
3:I:141:VAL:HG13	3:I:142:LYS:N	2.33	0.43
7:O:185:LEU:HD13	7:O:189:ALA:HB3	1.99	0.43
7:O:196:ASP:O	7:O:197:ALA:C	2.61	0.43
2:K:154:LEU:O	2:K:158:MET:N	2.52	0.43
3:I:102:LEU:HD23	3:I:102:LEU:C	2.43	0.43
7:O:42:ASN:O	7:O:46:GLN:HG2	2.18	0.43
7:O:60:LYS:HE2	8:P:48:SER:CA	2.49	0.43
7:O:67:VAL:CG1	7:O:72:ILE:HD11	2.48	0.43
9:T:928:ARG:HH11	9:T:931:LYS:HD3	1.83	0.43
12:D:35:LEU:HD22	13:B:53:ILE:HD12	2.01	0.43
14:G:30:DA:C2'	14:G:31:DT:H72	2.49	0.43
5:L:98:LEU:HD21	5:L:100:THR:OG1	2.18	0.43
8:P:219:LEU:HD12	8:P:219:LEU:N	2.33	0.43
3:I:200:ILE:HG22	3:I:201:CYS:N	2.34	0.43
8:P:164:LEU:HD23	8:P:169:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:897:TYR:CG	9:T:897:TYR:O	2.72	0.43
7:O:29:GLU:CB	7:O:32:LYS:HE2	2.49	0.43
7:O:29:GLU:CA	7:O:32:LYS:HE2	2.49	0.43
9:T:1014:VAL:HG12	9:T:1014:VAL:O	2.19	0.43
13:B:49:LEU:O	13:B:53:ILE:HG13	2.19	0.43
1:H:91:VAL:O	1:H:92:THR:C	2.62	0.43
9:T:970:HIS:ND1	9:T:1000:PRO:HB3	2.34	0.43
14:G:40:DG:H2"	14:G:41:DA:C8	2.54	0.43
15:J:30:DG:H2"	15:J:31:DC:H6	1.84	0.43
4:M:46:HIS:NE2	4:M:53:TRP:O	2.48	0.42
4:M:113:VAL:CG2	4:M:144:LEU:HD13	2.48	0.42
7:O:67:VAL:HG22	7:O:68:ARG:N	2.33	0.42
9:T:937:TYR:CE2	9:T:941:LYS:HD2	2.54	0.42
1:H:58:LYS:HB3	1:H:59:PRO:HD3	2.01	0.42
1:H:199:ILE:CB	2:K:147:LEU:HD21	2.49	0.42
2:K:213:MET:HE1	9:T:1005:PHE:CZ	2.53	0.42
3:I:393:VAL:HG21	3:I:401:LEU:HD11	2.02	0.42
3:I:623:LEU:O	3:I:626:VAL:HG23	2.19	0.42
5:L:99:ILE:HD12	5:L:99:ILE:N	2.34	0.42
6:N:10:LEU:HD23	6:N:10:LEU:O	2.20	0.42
7:O:47:LEU:CD1	8:P:31:ILE:HG23	2.50	0.42
9:T:932:LEU:HD12	9:T:935:THR:CG2	2.49	0.42
11:C:18:LEU:HD23	11:C:22:LEU:HD23	2.01	0.42
11:C:69:PHE:CD1	12:D:64:LEU:HD21	2.54	0.42
12:D:42:ILE:HG12	13:B:60:GLU:OE1	2.19	0.42
2:K:187:GLN:NE2	2:K:188:ILE:O	2.52	0.42
7:O:57:SER:OG	7:O:58:PRO:HD2	2.19	0.42
8:P:33:GLU:HG3	8:P:34:LEU:HD22	2.00	0.42
5:L:207:LEU:HD22	5:L:243:ILE:HD13	2.01	0.42
7:O:195:LEU:O	7:O:196:ASP:OD1	2.36	0.42
7:O:273:VAL:HG13	7:O:274:GLY:N	2.27	0.42
9:T:933:VAL:HA	9:T:936:ILE:HG12	2.01	0.42
12:D:18:ILE:HG13	13:B:32:LEU:HD21	2.00	0.42
1:H:105:LEU:HD23	1:H:105:LEU:O	2.20	0.42
3:I:320:ALA:HA	3:I:446:MET:HE1	2.02	0.42
5:L:226:THR:HG21	5:L:231:LEU:HD21	2.00	0.42
15:J:33:DG:H2"	15:J:34:DC:C5	2.53	0.42
1:H:31:GLY:HA3	8:P:42:TYR:CZ	2.54	0.42
3:I:386:ILE:O	3:I:390:VAL:HG23	2.20	0.42
7:O:249:LEU:HD12	7:O:252:GLN:HE21	1.85	0.42
10:A:69:LEU:N	10:A:69:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:85:LEU:HD22	4:M:96:ALA:HB2	2.01	0.42
4:M:100:LEU:HD21	4:M:139:ASN:HB3	2.02	0.42
8:P:12:THR:HA	8:P:15:LEU:CG	2.50	0.42
9:T:984:GLU:O	9:T:987:VAL:HG12	2.19	0.42
3:I:137:THR:O	3:I:141:VAL:HG12	2.20	0.42
6:N:157:VAL:HG22	6:N:168:PHE:HD1	1.84	0.42
7:O:30:ILE:HG21	8:P:16:GLU:OE2	2.19	0.42
8:P:17:LYS:HD3	8:P:17:LYS:HA	1.92	0.42
9:T:978:HIS:CB	9:T:986:ARG:HD3	2.49	0.42
9:T:982:PRO:HB2	9:T:984:GLU:CD	2.45	0.42
1:H:89:GLU:O	1:H:90:LYS:C	2.62	0.42
3:I:428:THR:O	3:I:432:ILE:HG12	2.20	0.42
9:T:906:THR:C	9:T:908:ARG:H	2.28	0.42
2:K:42:ASN:OD1	2:K:43:GLN:N	2.53	0.42
2:K:155:ILE:HD11	2:K:170:MET:HE1	2.02	0.42
2:K:165:LEU:O	2:K:166:ILE:C	2.62	0.42
2:K:196:ALA:O	2:K:205:ILE:HD11	2.19	0.42
6:N:61:ILE:HB	6:N:65:LEU:HD13	2.02	0.42
7:O:37:LEU:HB2	8:P:24:ILE:HD11	2.02	0.42
8:P:26:TYR:O	8:P:30:ARG:HG2	2.19	0.42
9:T:916:LYS:HD2	9:T:966:ILE:CD1	2.50	0.42
9:T:933:VAL:O	9:T:936:ILE:HG12	2.19	0.42
9:T:976:PHE:CD1	9:T:980:PHE:HD2	2.37	0.42
9:T:999:ILE:CG1	9:T:1000:PRO:HD2	2.50	0.42
11:C:13:ASP:OD1	11:C:14:LYS:N	2.52	0.42
14:G:31:DT:H2"	14:G:32:DT:C7	2.48	0.42
1:H:95:CYS:O	1:H:96:VAL:C	2.63	0.41
3:I:110:MET:CG	3:I:146:THR:HG21	2.49	0.41
6:N:167:LEU:HD22	6:N:199:ILE:HG23	2.02	0.41
1:H:128:LEU:HD21	2:K:79:PHE:HZ	1.85	0.41
3:I:161:ILE:HG21	3:I:181:LEU:HD22	2.01	0.41
9:T:895:LYS:CG	9:T:896:ARG:H	2.27	0.41
12:D:17:GLU:HG3	13:B:32:LEU:HD22	2.02	0.41
9:T:929:ALA:O	9:T:933:VAL:HG23	2.19	0.41
10:A:60:GLN:NE2	13:B:69:SER:O	2.53	0.41
6:N:315:ILE:H	6:N:315:ILE:HD12	1.85	0.41
8:P:13:LEU:HD12	8:P:16:GLU:OE2	2.20	0.41
9:T:909:LEU:HD23	9:T:910:TYR:H	1.84	0.41
15:J:24:DA:H2"	15:J:25:DA:H8	1.84	0.41
1:H:21:LEU:HA	1:H:24:VAL:CG1	2.51	0.41
6:N:26:VAL:HG23	6:N:27:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:106:LEU:C	6:N:106:LEU:HD23	2.45	0.41
6:N:107:ILE:HD13	6:N:134:LEU:HD11	2.02	0.41
7:O:45:PHE:HE2	7:O:49:ARG:HD2	1.84	0.41
6:N:44:ALA:HB3	6:N:46:LEU:CD2	2.51	0.41
6:N:110:LEU:O	6:N:114:ILE:HG22	2.20	0.41
7:O:83:ARG:HE	13:B:37:LEU:HD21	1.85	0.41
12:D:32:LEU:HD23	12:D:32:LEU:C	2.45	0.41
13:B:38:ILE:O	13:B:42:ILE:HG12	2.20	0.41
1:H:207:VAL:O	1:H:207:VAL:HG22	2.20	0.41
8:P:163:GLU:OE2	8:P:192:ARG:NH1	2.53	0.41
12:D:71:SER:O	12:D:74:VAL:HG22	2.21	0.41
9:T:890:LYS:C	9:T:892:LYS:H	2.29	0.41
9:T:905:THR:O	9:T:905:THR:HG22	2.21	0.41
14:G:37:DG:C2'	14:G:38:DT:H72	2.49	0.41
1:H:96:VAL:O	1:H:97:ALA:C	2.62	0.41
3:I:64:LEU:HD23	3:I:64:LEU:O	2.20	0.41
6:N:282:ILE:HD12	6:N:282:ILE:N	2.36	0.41
8:P:22:ASP:HA	8:P:25:VAL:HG12	2.02	0.41
9:T:916:LYS:HD2	9:T:966:ILE:HD13	2.03	0.41
9:T:957:LEU:O	9:T:961:MET:HG2	2.21	0.41
15:J:17:DT:H2''	15:J:18:DA:C8	2.56	0.41
2:K:80:LEU:O	2:K:83:ILE:HG22	2.21	0.40
2:K:164:ALA:O	2:K:165:LEU:C	2.64	0.40
4:M:148:ILE:O	4:M:148:ILE:HG22	2.21	0.40
6:N:71:ASN:OD1	6:N:72:ASP:N	2.53	0.40
6:N:5:ASN:OD1	6:N:5:ASN:N	2.54	0.40
7:O:34:ARG:CZ	7:O:34:ARG:HB3	2.51	0.40
9:T:820:MET:O	9:T:824:MET:HG2	2.22	0.40
9:T:891:TYR:O	9:T:892:LYS:C	2.65	0.40
10:A:33:ILE:HG12	13:B:45:ILE:HG12	2.03	0.40
1:H:92:THR:O	1:H:93:VAL:C	2.63	0.40
3:I:540:PHE:CD2	3:I:557:ILE:HD12	2.56	0.40
5:L:178:PHE:O	5:L:182:ASP:N	2.54	0.40
1:H:185:TYR:HD1	2:K:137:VAL:HG21	1.84	0.40
7:O:49:ARG:HE	12:D:45:SER:HB2	1.85	0.40
7:O:241:ILE:HG23	7:O:246:VAL:HG23	2.04	0.40
9:T:1012:HIS:O	9:T:1014:VAL:HG23	2.22	0.40
14:G:36:DC:H2''	14:G:37:DG:H8	1.81	0.40
14:G:38:DT:C2	14:G:39:DA:C5	3.10	0.40
2:K:54:ILE:CD1	4:M:178:ILE:HD12	2.51	0.40
5:L:207:LEU:HD12	5:L:207:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:817:LYS:HE2	9:T:817:LYS:CA	2.38	0.40
9:T:906:THR:OG1	9:T:908:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	224/239 (94%)	214 (96%)	10 (4%)	0	100	100
2	K	205/219 (94%)	200 (98%)	5 (2%)	0	100	100
3	I	577/661 (87%)	564 (98%)	13 (2%)	0	100	100
4	M	161/180 (89%)	157 (98%)	4 (2%)	0	100	100
5	L	229/302 (76%)	217 (95%)	12 (5%)	0	100	100
6	N	318/328 (97%)	307 (96%)	11 (4%)	0	100	100
7	O	252/325 (78%)	231 (92%)	20 (8%)	1 (0%)	30	48
8	P	279/638 (44%)	261 (94%)	18 (6%)	0	100	100
9	T	151/1016 (15%)	138 (91%)	13 (9%)	0	100	100
10	A	68/95 (72%)	68 (100%)	0	0	100	100
11	C	60/72 (83%)	60 (100%)	0	0	100	100
12	D	69/81 (85%)	68 (99%)	1 (1%)	0	100	100
13	B	53/82 (65%)	53 (100%)	0	0	100	100
All	All	2646/4238 (62%)	2538 (96%)	107 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	O	210	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	206/217 (95%)	204 (99%)	2 (1%)	68	83
2	K	189/198 (96%)	185 (98%)	4 (2%)	47	70
3	I	516/584 (88%)	513 (99%)	3 (1%)	78	89
4	M	147/161 (91%)	147 (100%)	0	100	100
5	L	218/277 (79%)	218 (100%)	0	100	100
6	N	285/290 (98%)	285 (100%)	0	100	100
7	O	228/295 (77%)	226 (99%)	2 (1%)	70	84
8	P	255/579 (44%)	252 (99%)	3 (1%)	63	80
9	T	144/942 (15%)	140 (97%)	4 (3%)	38	62
10	A	64/89 (72%)	64 (100%)	0	100	100
11	C	56/66 (85%)	56 (100%)	0	100	100
12	D	65/75 (87%)	65 (100%)	0	100	100
13	B	52/76 (68%)	52 (100%)	0	100	100
All	All	2425/3849 (63%)	2407 (99%)	18 (1%)	73	88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	189	LEU
1	H	198	MET
2	K	138	LYS
2	K	147	LEU
2	K	158	MET
2	K	212	LYS
3	I	147	LEU
3	I	182	LEU
3	I	560	LEU
7	O	185	LEU
7	O	196	ASP
8	P	250	GLU

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Mol	Chain	Res	Type
8	P	259	LYS
8	P	265	LYS
9	T	815	ILE
9	T	910	TYR
9	T	938	HIS
9	T	977	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	12	GLN
1	H	215	ASN
2	K	172	GLN
3	I	93	GLN
3	I	591	GLN
3	I	612	HIS
4	M	134	ASN
4	M	139	ASN
4	M	177	ASN
5	L	189	GLN
6	N	313	HIS
7	O	27	GLN
7	O	42	ASN
7	O	54	HIS
7	O	233	GLN
7	O	252	GLN
8	P	76	GLN
8	P	80	GLN
8	P	266	GLN
10	A	8	GLN
11	C	33	GLN
11	C	45	ASN
11	C	52	ASN
12	D	43	ASN
12	D	72	HIS
13	B	55	HIS
13	B	68	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

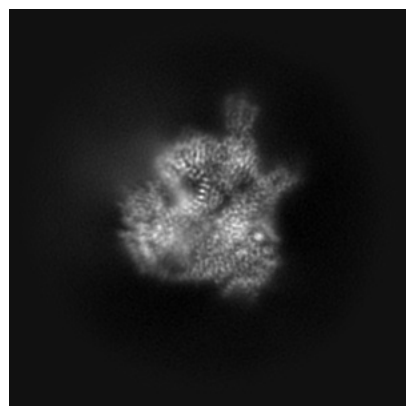
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70560. These allow visual inspection of the internal detail of the map and identification of artifacts.

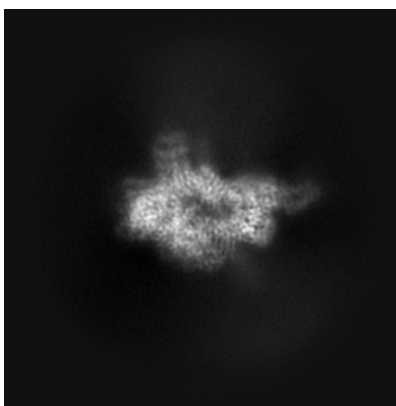
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

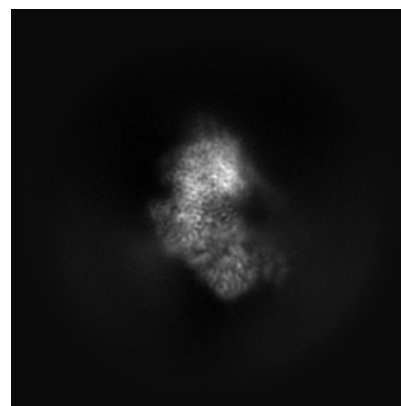
6.1.1 Primary map



X

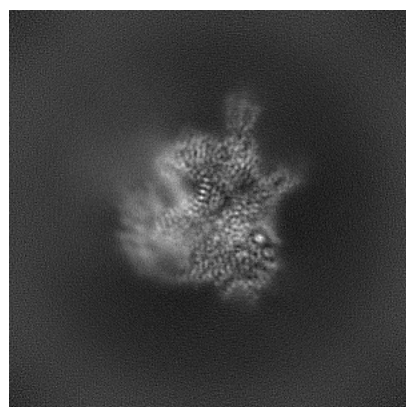


Y

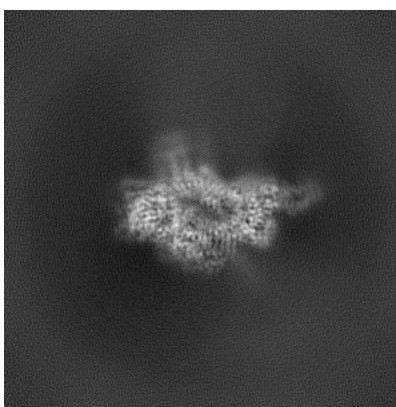


Z

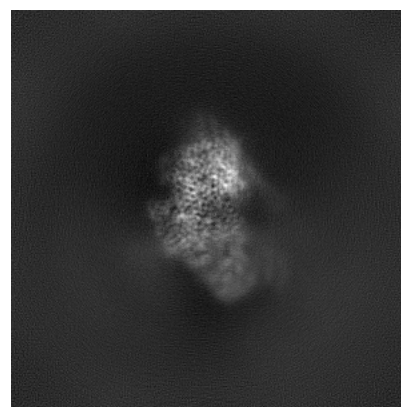
6.1.2 Raw map



X



Y

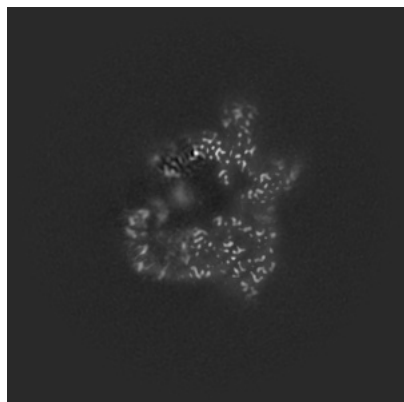


Z

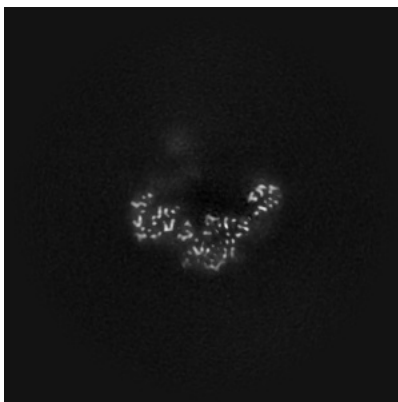
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

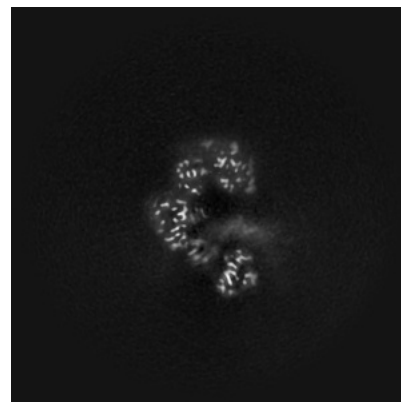
6.2.1 Primary map



X Index: 213

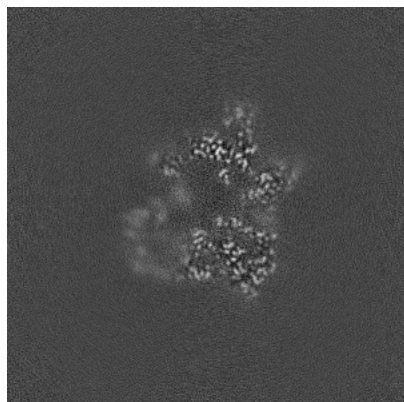


Y Index: 213

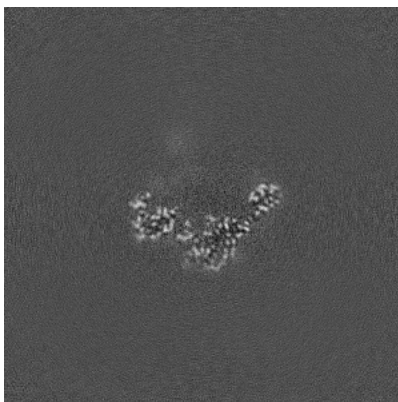


Z Index: 213

6.2.2 Raw map



X Index: 210



Y Index: 210

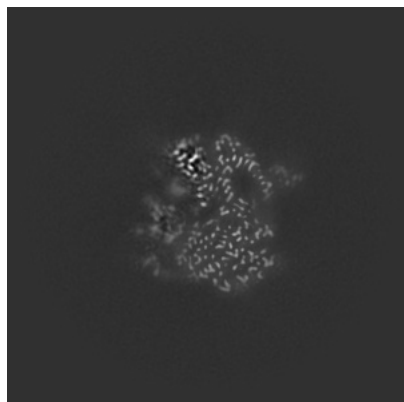


Z Index: 210

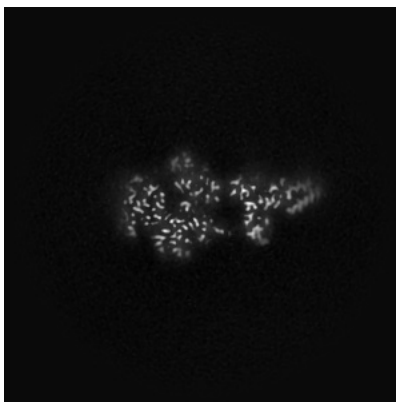
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

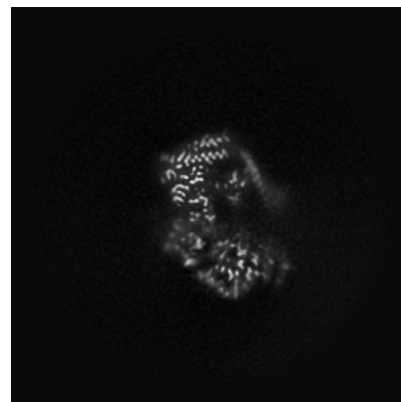
6.3.1 Primary map



X Index: 197

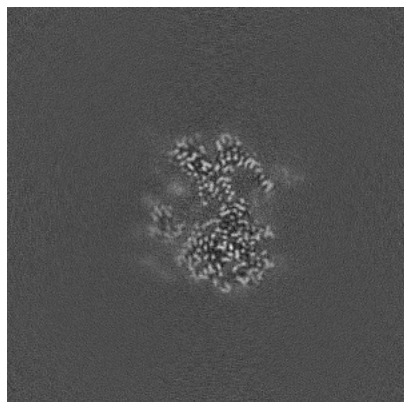


Y Index: 247

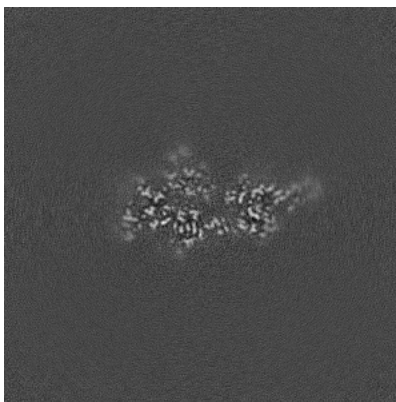


Z Index: 183

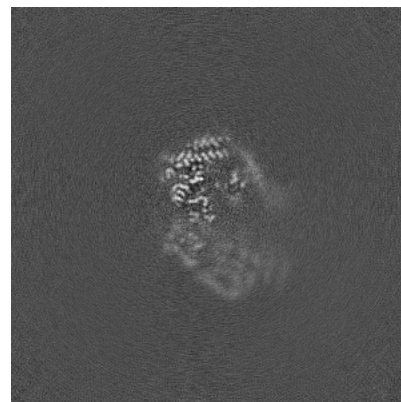
6.3.2 Raw map



X Index: 193



Y Index: 235

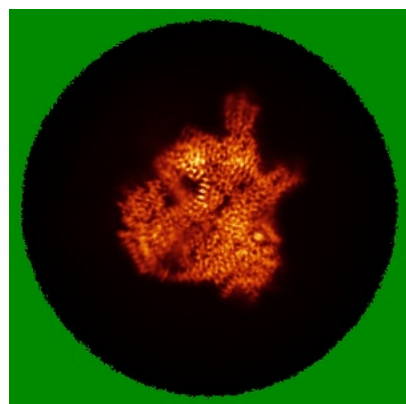


Z Index: 180

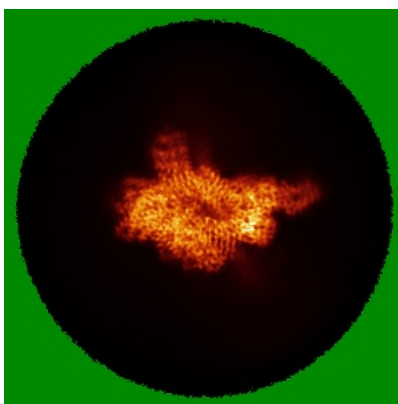
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

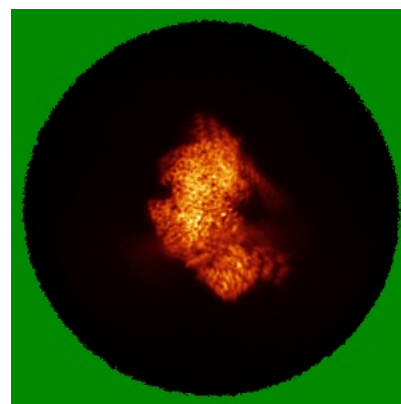
6.4.1 Primary map



X

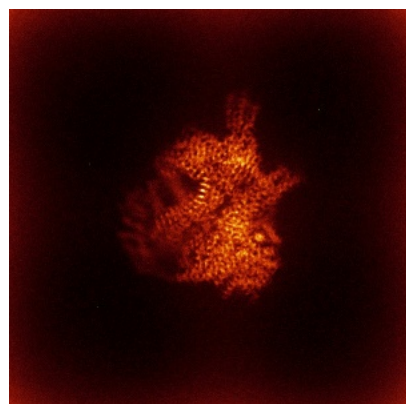


Y

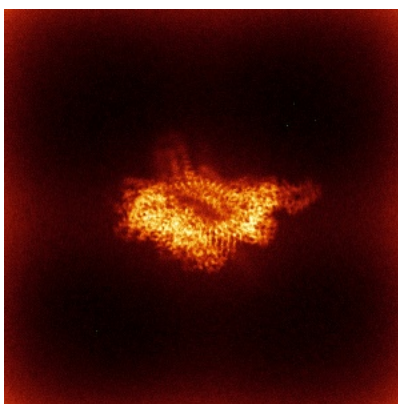


Z

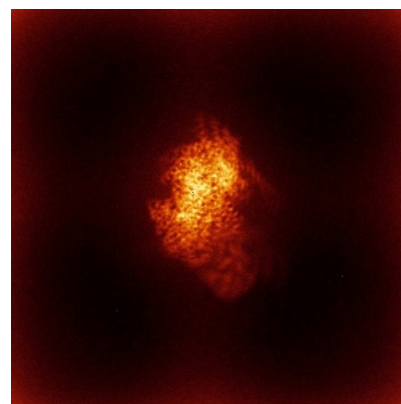
6.4.2 Raw map



X



Y

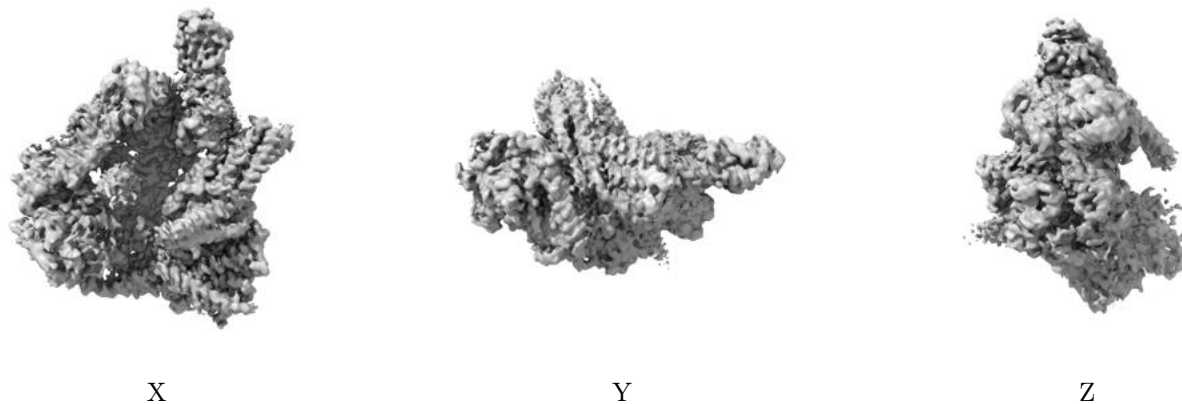


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

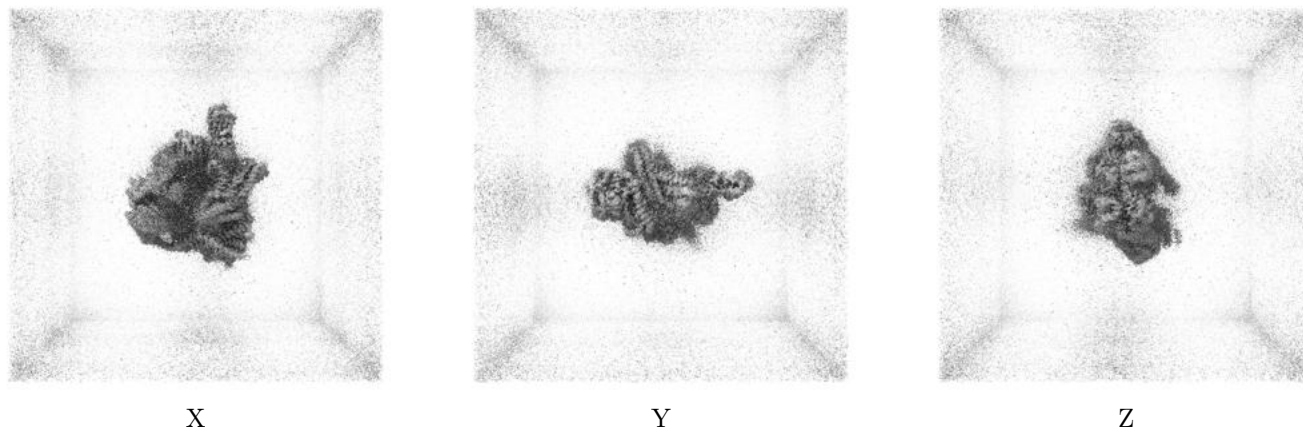
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0332. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

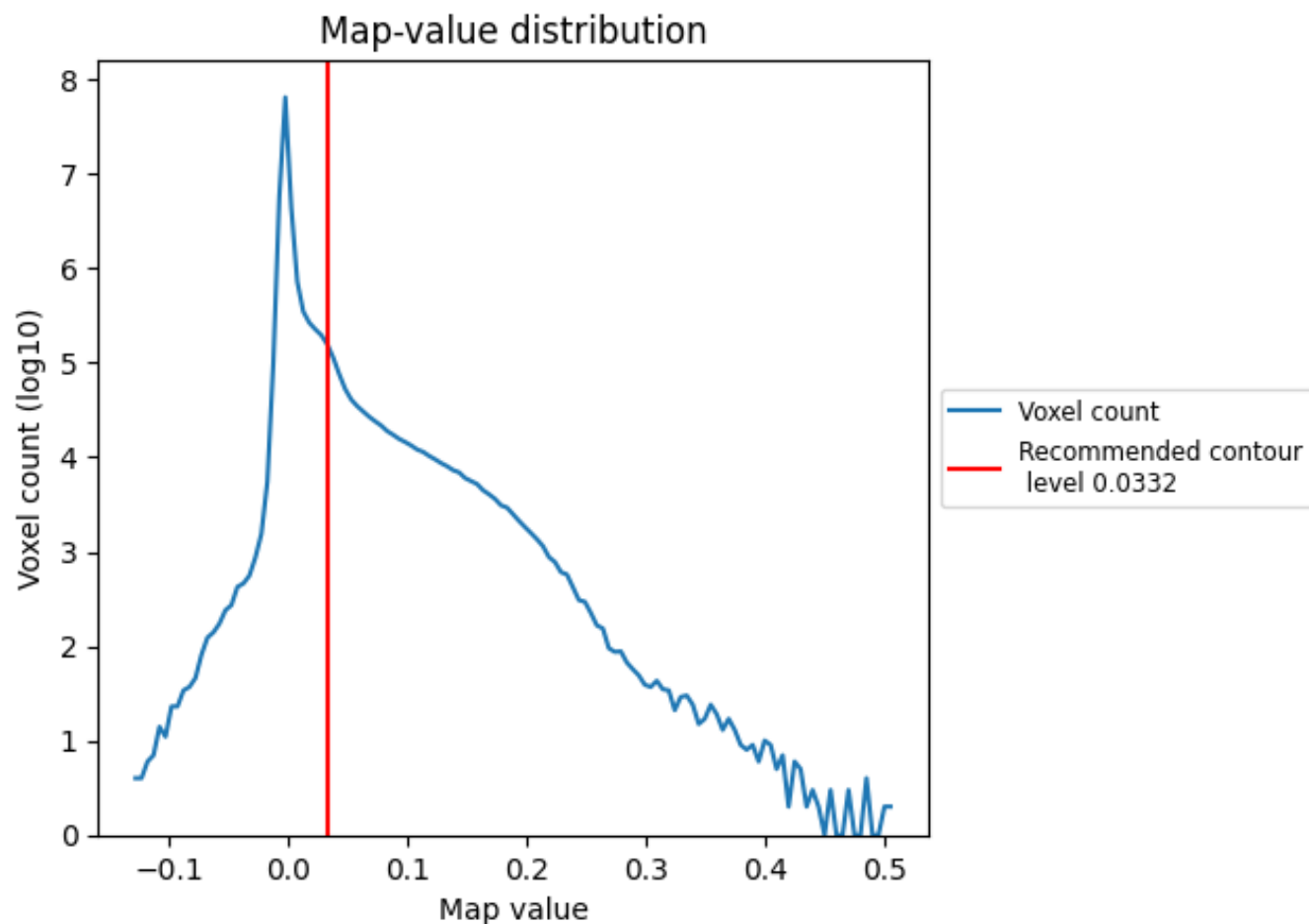
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

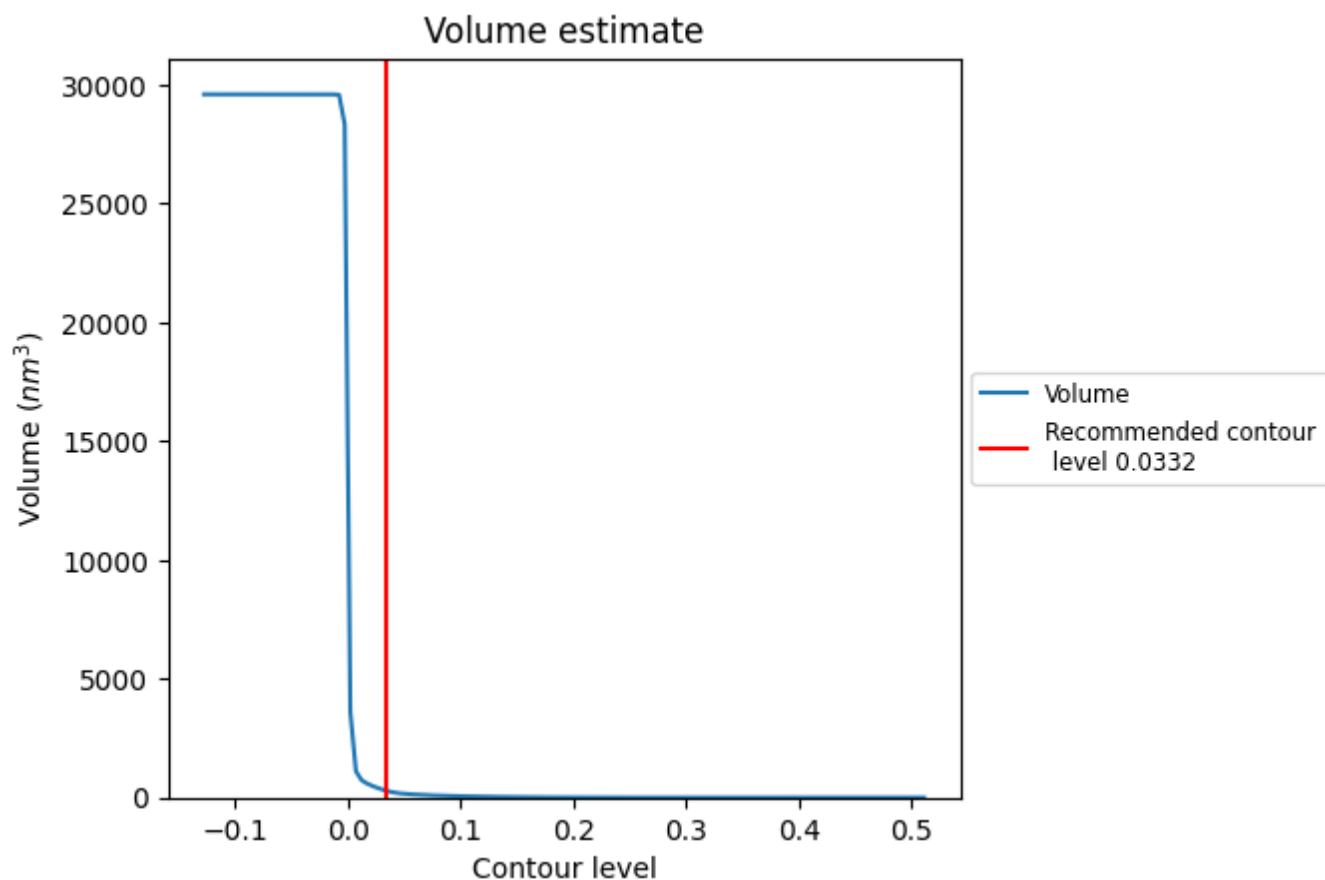
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm³; this corresponds to an approximate mass of 270 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

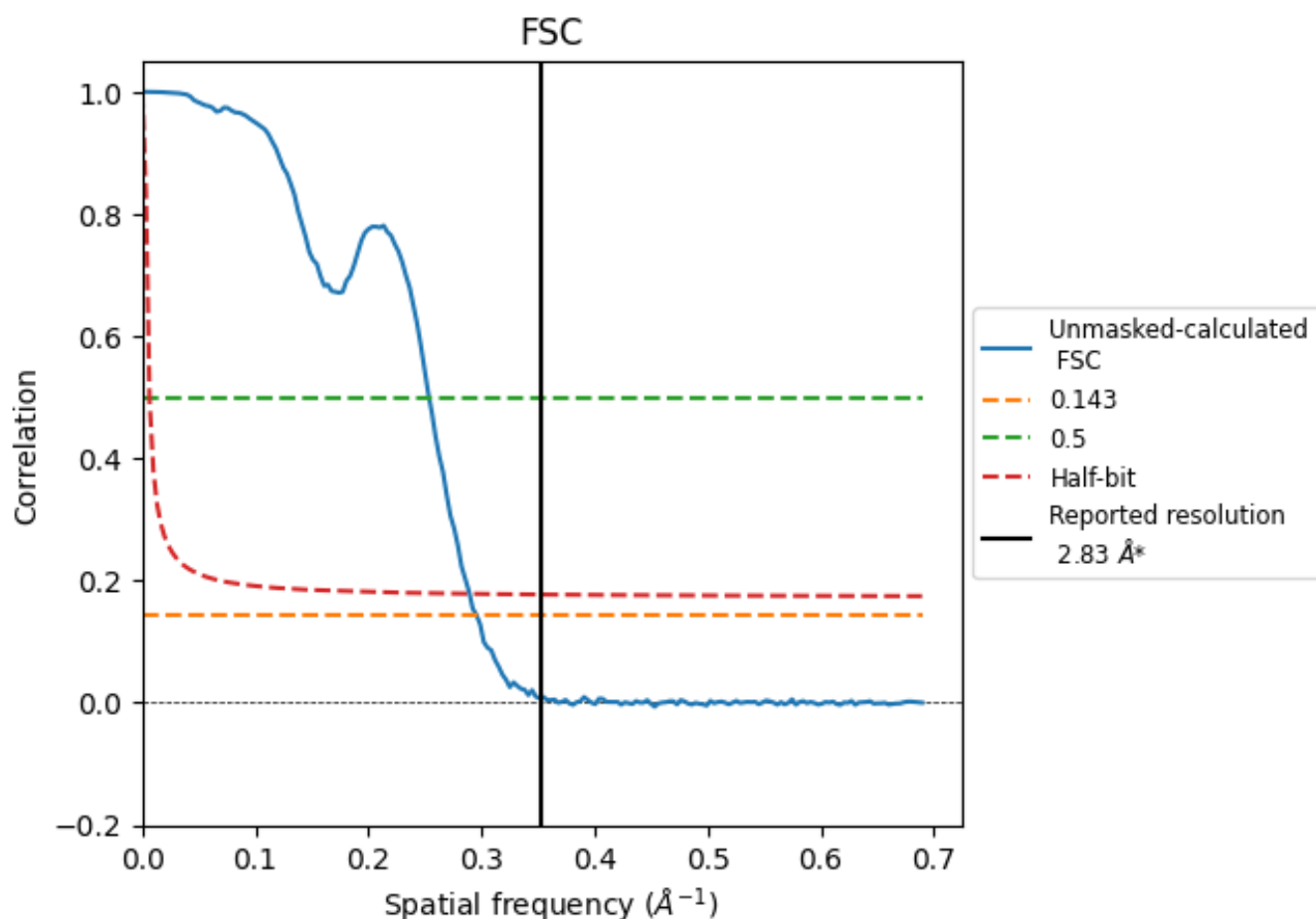
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

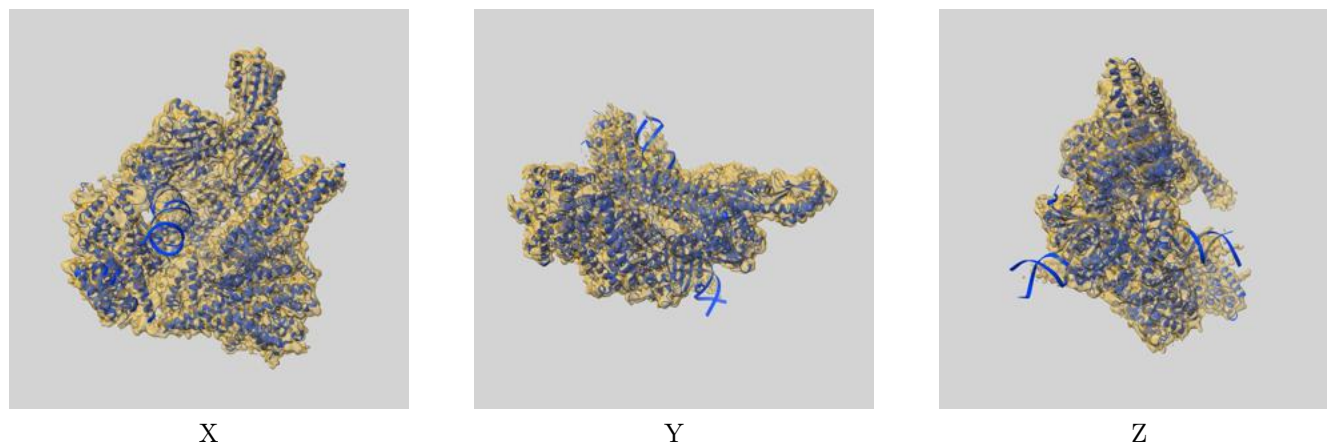
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.94	3.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.38 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

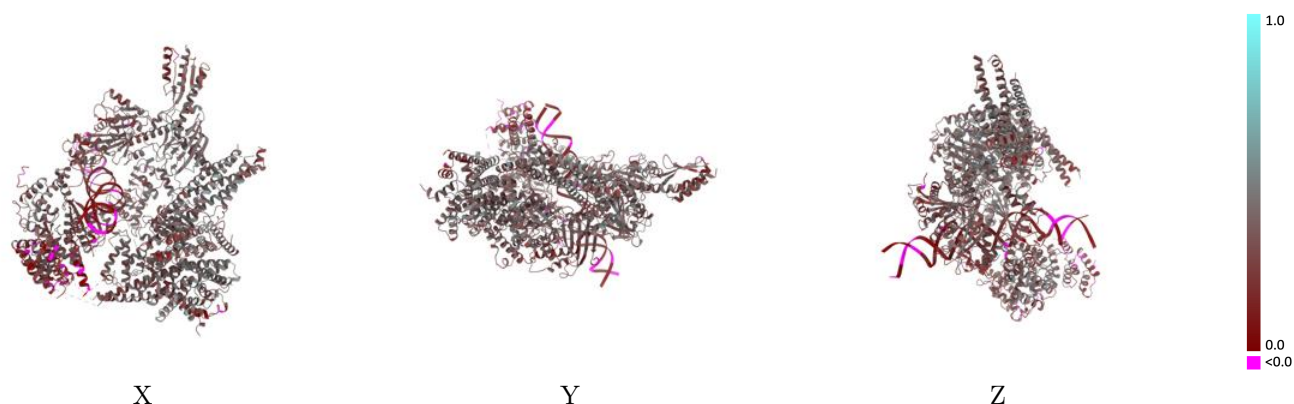
This section contains information regarding the fit between EMDB map EMD-70560 and PDB model 9OKD. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



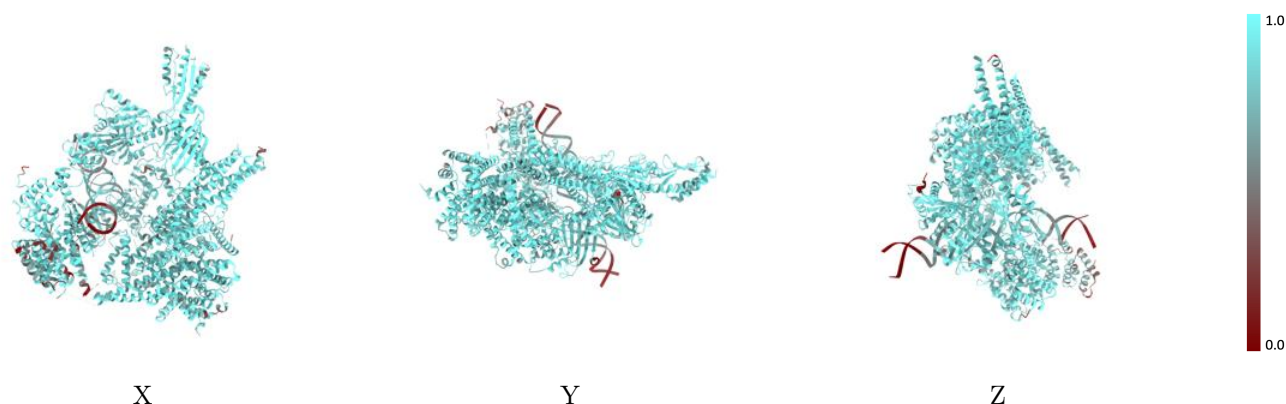
The images above show the 3D surface view of the map at the recommended contour level 0.0332 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



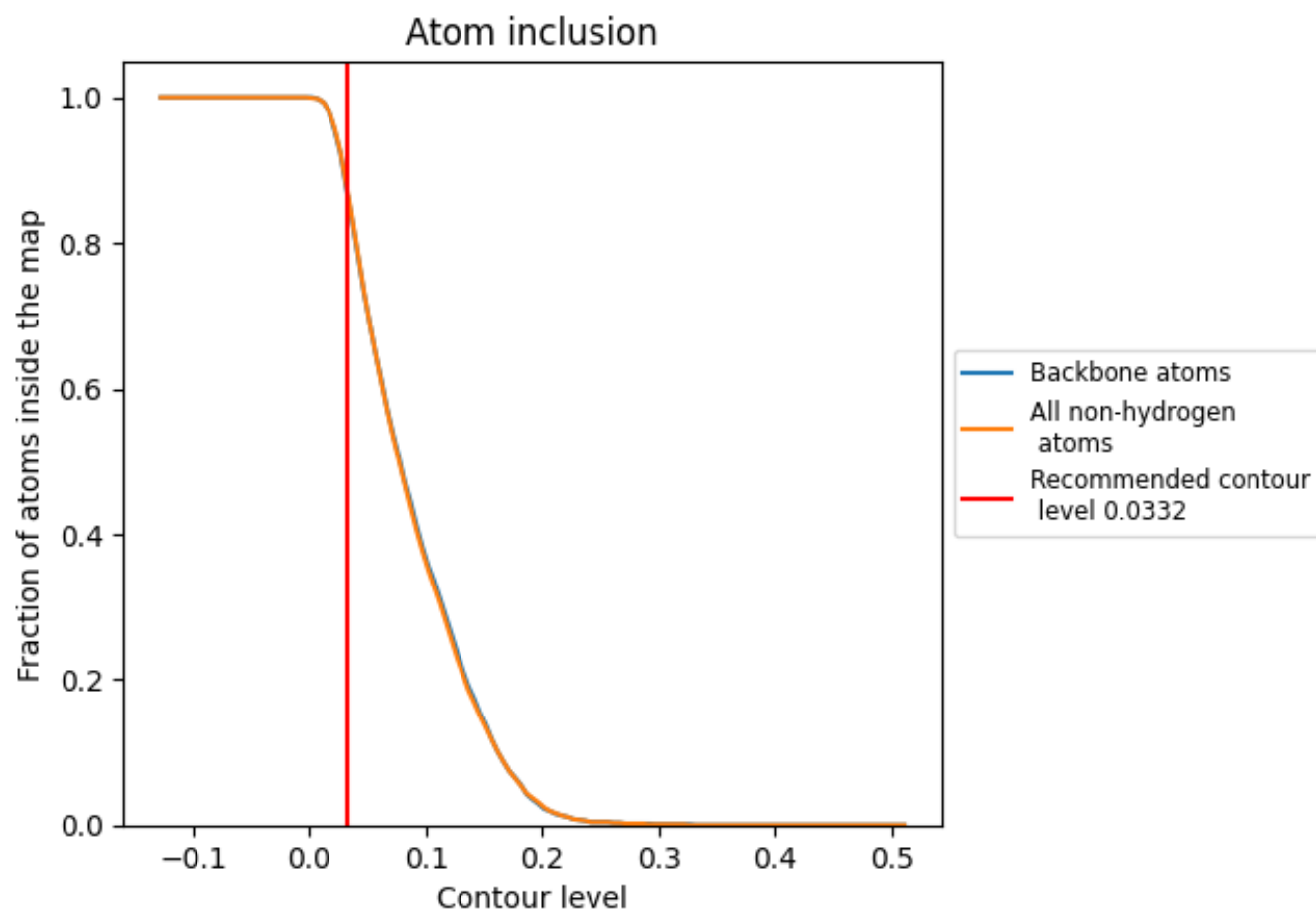
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0332).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0332) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.3310
A	 0.8790	 0.3660
B	 0.9520	 0.4070
C	 0.8500	 0.3860
D	 0.9460	 0.4070
G	 0.5060	 0.0890
H	 0.9260	 0.3700
I	 0.8650	 0.3310
J	 0.5370	 0.0950
K	 0.8990	 0.3230
L	 0.8970	 0.2720
M	 0.9370	 0.3950
N	 0.8800	 0.3500
O	 0.9230	 0.3630
P	 0.8900	 0.3580
T	 0.8730	 0.3540

